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COMPUTER CONTROL OF CHEMICAL PROCESS PLANTS WITH SPECIAL REFERENCE TO DISTILLATION

A Thesis submitted for the degree of

Doctor of Philosophy

by

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Computer Control of Chemical Process Plants with Special Reference to Distillation

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SUMMARY

A sieve plate distillation column has been constructed and interfaced to a minicomputer with the necessary instrumentation for dynamic, estimation and control studies with special bearing on low-cost and noise-free instrumentation.

A dynamic simulation of the column with a binary liquid system has been compiled using deterministic models that include fluid dynamics via Brambilla's equation for tray liquid holdup calculations. The simulation predictions have been tested experimentally under steady-state and transient conditions. The simulator's predictions of the tray temperatures have shown reasonably close agreement with the measured values under steady-state conditions and in the face of a step change in the feed rate.

A method of extending linear filtering theory to highly nonlinear systems with very nonlinear measurement functional relationships has been proposed and tested by simulation on binary distillation. The simulation results have proved that the proposed methodology can overcome the typical instability problems associated with the Kalman filters. Three extended Kalman filters have been formulated and tested by simulation. The filters have been used to refine a much simplified model sequentially and to estimate parameters such as the unmeasured feed composition using information from the column simulation. It is first assumed that corrupted tray composition measurements are made available to the filter and then corrupted tray temperature measurements are accessed instead. The simulation results have demonstrated the powerful capability of the Kalman filters to overcome the typical hardware problems associated with the operation of on-line analyzers in relation to distillation dynamics and control by, in effect, replacing them.

A method of implementing estimator-aided feedforward (EAFF) control schemes has been proposed and tested by simulation on binary distillation. The results have shown that the EAFF scheme provides much better control and energy conservation than the conventional feedback temperature control in the face of a sustained step change in the feed rate or multiple changes in the feed rate, composition and temperature.

Further extensions of this work are recommended as regards simulation, estimation and EAFF control.

Key Words

Control, distillation, simulation, estimation, feedforward, interfacing

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Dedicated to Janet

and also

to the memories of a, once fluid, man, crammed and distorted by classical mess .....

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C H A P T E R O N E

INTRODUCTION

C H A P T E R T W O

LITERATURE REVIEW

Control, Simulation and Filtering

I.1 REASONS FOR THE STUDY OF DISTILLATION CONTROL

There exist many cogent reasons for interest in the control of distillation columns.

Primarily, distillation columns constitute an important part of many industrial processes - frequently the last separation unit in the process. Therefore, the quality of the product leaving the entire process depends on the quality control of distillation operation. Occasionally, they are vital intermediate units on the constancy of whose products depends the consequential ease of control of succeeding units such as reactors.

Secondly, sufficient available knowledge about the physical nature of distillation enables the creation of reasonably successful static and dynamic mathematical models. The degrees of sophistication of these models are no longer major drawbacks as powerful digital computers can cope with the calculations almost regardless of volume or complexity. Thus, having dispensed with the modelling problems, more attention can then be focussed on the control aspects of distillation columns. The implication of this, however, is not that the understanding of distillation as a physical process is complete; outstanding issues such as fluid dynamics and the efficiency of separation on the plates are still not well established and require further research.

Thirdly, the problems encountered in the control of an average continuous distillation column are similar to the typical problems of chemical process control,

the status of which has been the subject of considerable controversy and criticism in recent years.

Finally, the reward for reducing off-specification product in terms of energy saving and economy of operation is, presently, increasing by the day. Although we are living in an ever changing world, it can be confidently asserted that, no matter what the future holds, the cost of production of any commodity will continue to escalate and, therefore, the most effective way to maintain profitability must be to reduce wastage. By the token that energy is the currency of nature regardless of time and distillation may certainly be very wasteful of it, its economical use becomes imperative in relation to distillation.

The literature contains various reports which show that the energy savings of a chemical plant have been enhanced by no less than a half by implementing good control on distillation columns.

The last reason has materialized concurrently with the recent energy crisis and, although more materialistic than academic, can be regarded as the most powerful argument in favour of distillation column control - an incentive that will continue to gain momentum as energy becomes less and less available.

On the other hand, good control of distillation columns by conventional methods is not easy and has been the subject of much research lately. Precise control is difficult to achieve conventionally because:

(i) columns with many trays exhibit slow response to control action.

(ii) separation is affected by many variables requiring many control loops that interact with one another.

(iii) on-line analysis is not always available.

(iv) distillation units are usually the last in the chain of processing units and are, therefore, subject to changes in throughput from all upstream units.

(v) the factors affecting separation are not readily interpreted in terms of control system requirements.

In view of these problems, the conventional control methods that will be reviewed later in this dissertation have met with limited success and even a lesser degree of generality on application to distillation columns.

To conclude, it only remains to reiterate that the challenge of distillation column control, although formidable, continues to be extremely attractive.

I.2 REVIEW OF THE DEVELOPMENTS OF THE CONTROL THEORY AS APPLIED TO DISTILLATION

Up until the early sixties there was no standard method of controlling distillation columns and no system had been found capable of forcing a column to behave as the designer had intended. But then a revolution began and, for the past two decades, various groups working independently have been apparently making strides in the areas of the dynamics and control of distillation columns.

Although the published work is extremely diversified, broadly speaking, three distinct paths can be identified in the developments made in these areas which are namely:

1. The deductive path
2. The mathematical path
3. The computer path

Admittedly, the computer and the mathematical paths do overlap to some extent in that they are in effect complementary. Nonetheless, they will be treated separately in order to contrast and better elucidate them. The computer path would perhaps be better worded as a mathematical path to which the computer is an indispensable tool. Completion of any control configuration in any process control practice comprises two stages:

1. The analysis of the control problem which includes detailed study of the dynamics of the process under consideration.
2. The synthesis of the control strategy including

stability studies.

Computers can be an important tool in both stages. In this capacity, they have affected the development of control theory in the following ways:

1. They have enabled complicated solutions to be synthesized by the use of computer aided design techniques.
2. They have enabled complicated control configurations to be implemented.

Additionally, there has also been some development of ideas through experimentation but this has been limited because the verification of control strategies by experimentation is usually only valid for the specific cases under consideration.

The deductive path, as reflected in the work of Shinskey and co-workers (17,18,31,32) by-passes the first stage and avoids the problem of dynamics completely and is purely based on observations and experience. It is characterised by the logical arrangement of arguments and observations to detect regularities of behaviour without too much recourse to formulae.

The concept of material balance control which appears to be the most industrially acceptable control method falls into this category. It is essentially a system designed to hold the process in dynamic equilibrium - notwithstanding variations in throughput and environmental conditions - by reducing the interaction between the column's heat and material balances. Further, heuristics are introduced for coupling the manipulated

and the controlled variables which are then treated as single-loop systems and analysed by classical control theory. The resulting control scheme is then implemented by conventional hardware.

On the one hand, classical control theory suffers from the inability to handle non-linearities and to guide the control system design for a dynamically interacting multivariable process such as distillation. On the other hand, the literature contains no evidence as to how far-reaching these rules of thumb may be. Therefore, the scepticism about such a simplistic approach may not be totally unjustified. The margin between sophistication and sophistry is always narrow in deduction and inference and there can be few subjects where the risk of developing into an armchair philosopher is greater than it is in distillation dynamics and control.

The followers of the mathematical path, however, have approached the problem more realistically and with inspired thought inasmuch as they have acknowledged the multivariable nature of the distillation control problem. Modal control proposed by Rosenbrock (33) and various attempts to apply feedback and feedforward control belong to this class, all of which are direct translations of control techniques employed elsewhere except modal control which has an air of novelty around it. An excellent exposition of modal analysis and some useful examples are given by Gould (23). These techniques will be reviewed in more detail in Chapter II.

The main feature of the mathematical path is the

fact that it is essentially concerned with deriving equations to describe an individual stage in the Laplace or time domains and stepping this up from a single stage to a column with a number of similar stages. The dynamics are then studied and control configurations are specified by solving the control problem analytically or numerically. For example, in application of optimal feedback control to a binary distillation column the matrix Ricatti equation as used by Jordan (25) had an analytical solution proposed by Walter (26).

It is also of interest to note that in contrast to the deductive path that aims at minimising interaction, the mathematical path usually advocates the exploitation of interactions as in the case of modal control.

The amount of detail that should be included in these mathematical models to make them realistic representations of the phenomena occurring in distillation columns is, nevertheless, not clear-cut and yet another major shortcoming of the mathematical path is due to its inability to guard against the practical problems of the implementation of the derived control strategies. These problems are highlighted in unknown disturbances, non-linearities, inherent measurement errors, lack of availability and infrequency of primary control measurements.

Despite the upsurge of enthusiasm for the mathematical path that followed the introduction of modal

control by Rosenbrock (33), the interest in this path appears to have subsided and very few cases are reported in the literature that are indicative of any potential progress in the application of such techniques to distillation control. To some extent, this is the reason why control practitioners are rarely interested in the mathematical path - especially in the industry.

This lack of progress, however, is thought to be partly due to the inherent amount of calculation involved in such approaches which in many cases may prove to be prohibitive particularly in multicomponent distillation. Yet another obstacle has been the practical problems of implementation of the consequential control strategies. For instance, for this very reason any successful demonstrations that multivariable control can, indeed, achieve superior results to the conventional single-loop approach may have been hampered.

In other words, although the theory is good, it has failed to achieve the deserved results in practice for the reasons mentioned above.

The advocates of the computer path have, however, shown more signs of life. A few workers such as Brosilow and Weber (34), encouraged by the increasing availability of computers especially for on-line prediction of dynamics and control, have made better use of them to study more realistic situations. They have faced facts concerning model inaccuracies, unknown disturbances and the scarcity of reliable primary measurements : and to overcome these problems, they have

proposed the use of various optimal or sub-optimal static or dynamic estimators.

More recently, the on-line use of digital computers for data acquisition and control has been advanced. With the increasing availability of high speed digital computers and the advent of micro-processors, they should continue to consolidate their position as an accepted tool of the trade.

I.3 THE ROLE OF THE COMPUTER

In a retrospect of the past two decades of distillation column control the conclusion is inescapable that any approach to control that does not include the prediction of the dynamic behaviour of the column will not suffice. The prediction of the dynamics of a complex process of a high dimensionality such as distillation cannot be accomplished effectively without a computer since the sheer volume of calculations needed for even a small column makes it humanly impossible to cope with.

On the control front, for example, using optimal control theory to develop a controller would involve a feedback matrix relating the state vector to the vector of the manipulated variables. Needless to say the ease of implementation of such a system on a computer is more attractive than implementation by hardware. Further, this matrix may even be time variant which would confuse the issue even more when conventional hardware is used. Not only may the computer be cheaper, but it would almost certainly be easier to implement.

Continuing in this context, the computer can greatly assist the examination of the past record to find the best conditions in which the process should run, particularly when different shifts operate a column in different fashions - the computers are not solely controllers and may act as data-loggers which produce information that may be of use for more productive use

of the column.

In the previous section, it was stated that precise control is, in practice, marred by noisy or corrupt measurements. The only way to refine these measurements, and thereby improve control, is by stochastic estimation methods - whether they be primary or secondary measurements - and this is not a difficult task for an on-line computer. Indeed, in this capacity, the role of the computer as an aid to control can hardly be equalled.

Sadly, while computers have become widely accepted as control aids in industries such as the steel industry, they do not appear to have achieved the same level of recognition in the chemical industry. But at long last this picture has begun to change over the past five years with the dramatic decrease in the cost of computers that has eliminated the economic deterrent against their use. The other major obstacle, however, lies in the fact that, in chemical industries, there are frequently fire hazards which necessitate the use of non-electrical or heavily-proofed elctrical measurement and valve systems. Digital computers require electrical inputs and this means that either pneumatic-electric convertors or heavily proofed electrical systems must be utilized. A large part of the problem in interfacing computers to chemical processes is due to the fact that the electrical signals to the actuators on the plant and from measurement devices may have to satisfy stringent demands which are costly

to comply with. It might be that extensive research into interfacing chemical plants to computers would produce a significant drop in the cost of on-line computers.

To sum up, despite the remaining problems of interfacing that should be removed in time, the increasing complexity of chemical process industries and the speed at which decisions need to be made should promote the extensive use of high speed digital computers to help the engineers in the estimation and control of the states of the systems.

I.4 THE ROLE OF SIMULATION

Yet another impetus for the use of high speed digital computers as an aid to design and control of chemical processes stems from the growing tendency towards a more quantitative approach to problems of design and control, inasmuch as powerful computers can be of great value in solving complex systems of mathematical equations statically or dynamically - equations that would have been impossible to solve analytically.

Generally speaking, as regards distillation columns, or any process plant, simulation can be subservient to engineers in the following ways:

(i) alternative designs can be sought to achieve more efficient and optimal operation of existing plants

(ii) dynamic and static characteristics of future plants can be predicted and optimized

(iii) the computerized analytical approach provides a deeper understanding of the internal mechanisms of the processes studied

(iv) different control schemes can be tried rapidly and economically on a simulation instead of the alternative time-consuming tests on the actual or pilot plants

All these factors, viewed collectively, culminate in describing simulation as an effective technique of improving the profitability of an existing or proposed

design.

In a world ever conscious of costs and profits, every technique which helps to improve efficiency must be considered; simulation provides some of the important methods for achieving these objectives.

The pioneering works of Franks (2), Ramirez (5), Luyben (3) and Robinson (4) have gone a long way to introduce and establish this important tool for chemical engineering practice. The work of Kocak (36) on dynamic simulation of chemical plants is another example of the growing interest in this area. No doubt interactive simulation should follow suit and extend the flexibility and the horizons of the process simulation even further to make it more fascinating.

In relation to this thesis, simulation has been used to serve the following purposes:

1. To study the dynamic behaviour of a binary distillation column.
2. To explore the possible functions to be fulfilled by the Kalman filter.
3. To test control configurations prior to implementation on the column.

I.5 THE ROLE OF ESTIMATION

Control is mainly concerned with decision making and therefore taking action to counteract any undesirable disturbance that might have an adverse effect on the state of a physical system.

Pre-requisite to making timely and expedient decisions are the availability of reliable information about the system, the nature of the disturbances and the way in which these disturbances are manifested in the system - i.e. the response of the system.

As regards chemical processes, in the face of a disturbance, one might wait for the effect to manifest itself in the system, measure the magnitude of the effect and then take appropriate corrective action, which is commonly known as feedback control. Alternatively, one could choose to anticipate the effect of the disturbance by a mathematical description of the physical system and, in theory, nullify the effect before it materializes - in other words feedforward control.

Occasionally a combination of these two techniques is used to increase the chances of success in controlling the state of the system. Whatever the philosophy of control may be, two sources of information are available to the engineer; these are, namely, the measurements of the process variables and a mathematical description of the physical system based on physico-chemical laws. In chemical engineering systems these are both subject to errors.

To succeed in controlling a system, some information about the state of the system is necessary. In fact, mathematical descriptions and measurements may be regarded as being the tools of acquiring such information. In a real chemical engineering system which is subject to disturbances there is a true state which will never be known exactly and a few variables which can be measured only inaccurately because of noises in the measurement instruments and in the communication channels. Invariably, the mathematical description of the system is also inaccurate.

The problem of accurately determining the state of a system from noisy measurement is called estimation or filtering. It essentially involves recovering reliable information from corrupt measurements and, optionally, combining the recovered information with the predictions of a mathematical model to provide the "best" estimates of the state of the system (e.g. Kalman filtering). In 1960, Kalman (35) extended the filtering theory to cover the estimation of the states described by a set of linear differential equations and following this development, the classical Kalman filter has been applied in many diverse fields, in particular in the aerospace industry. More recently, the extended version of the Kalman filter has been proposed to deal with non-linear systems.

The following broad classes of problems require estimation techniques:

(i) the determination of model parameters in non-linear algebraic models from experimental measurements.

(ii) the off-line determination of model states in non-linear dynamic models from time-sampled experiments.

(iii) the on-line modelling of dynamic processes where sampled output signals are used to generate estimates of the states and parameters in process models.

The techniques involved in the second and third classes of problems are classified as non-sequential or sequential estimation. In the sequential approach estimates of state variables and parameters are generated at each sampling instant. The non-sequential approach is based on taking a series of samples over a period of time.

A sequential approach to estimation is commonly referred to as recursive filtering because current state and parameter estimates are calculated as the output measurements become available; hence one is continuously filtering the system. The recursive filtering problem can thus be identified as the estimation of the current states of a dynamic system using all the past and present measurements without the necessity of storing the past measurements.

Another significant application of estimation in chemical engineering is in relation to control and emerges in the form of estimating product quality from secondary process measurements. For instance, in

distillation columns a corrupt temperature measurement may be used to estimate the composition on a plate where equilibrium conditions may not necessarily be prevailing - i.e. the filter functions as an on-line analyzer.

As far as estimation is concerned, its application in off-line and on-line modes are investigated in this research. In an off-line capacity, an extended Kalman filter is used to sequentially refine an inaccurate model and estimate parameters such as feed rate and feed composition using information from the column simulation which is known to be reasonably accurate. It is first assumed that compositions are available directly and then plate temperature measurements are accessed instead. In an on-line mode, the role of the estimator is much the same as the off-line case except that the column simulation can be replaced by the actual column and a mini-computer can be employed for real-time data acquisition, estimation and control.

I.6 THE ROLE OF FEEDFORWARD CONTROL

Without loss of generality, one can say that the feedback control method has been the traditional method of controlling distillation columns in the industry. It often provides acceptable control despite scant knowledge of the dynamic character of the column. However, corrective action is taken only after the product qualities have deviated from their desired values, and long times are often required to bring the unit back to the desired steady state, especially in large towers. This can be considered as being a defensive attitude.

We live in an era in which economic constraints are making survival increasingly difficult in any area. Therefore, common sense dictates that we cannot afford the expensive luxury of waiting for things to go wrong before taking any counter measures. A deviation in product quality, when it occurs, is already costly. Indeed, man has much to gain in the game of economic survival by anticipating the adversities and taking counter measures before his system is disturbed. Feedforward control is compatible with this school of thought. It is heartening to know that this fact has been acknowledged in chemical process industries in the past decade and feedforward control systems have gained wide acceptance in chemical engineering systems. They have demonstrated their ability to improve control, sometimes quite spectacularly (Luyben (3)). It is indubitably a

control philosophy that is more relevant to chemical engineering systems than any other engineering fields. Our systems are often slow-moving, multivariable and contain appreciable dead times. All these characteristics can make life awkward for feedback controllers whereas feedforward controllers can handle them with relative ease.

The basic notion of feedforward control is to detect the disturbances as they enter the process and make adjustments in the manipulated variables so that the output variables are held constant. One does not wait until the disturbance has worked its way through the process and disturbed everything to produce an error signal. If a disturbance can be detected as it enters the process, it makes sense to take immediate action in order to compensate for its effect on the process.

In application to chemical processes, feedforward control usually suffers from the following limitations:

1. Inexact mathematical or empirical models are used to predict the dynamic behaviour.
2. Changes in controlled variables caused by unknown or unmeasured disturbances may go uncorrected.

It is argued in this thesis that the dyad of a Kalman filter and feedforward control scheme should overcome these problems.

I.7 THE OBJECTIVES OF THIS THESIS

This thesis is concerned with a research project whose prime objective is to carry out investigations into the computer control of chemical process plants with special reference to the control of distillation columns. It essentially comprises the following stages:

(i) the construction of a distillation column with the necessary instrumentation and its interfacing to the Honeywell-316 computer with special bearing on cheap and reliable methods of level, flow and temperature measurements that are sufficiently accurate and immune from noise.

(ii) the dynamic simulation of binary distillation columns employing a model that incorporates fluid dynamics in a realistic and easy-to-handle fashion in the form of plate liquid holdup calculations.

(iii) the exploration of the dynamics of the distillation column and comparison of experimental results with the predictions of the simulation.

(iv) application of an extended Kalman filter to the column simulation in an effort to demonstrate the use of Kalman filter for model refinement.

(v) estimation of tray compositions from secondary measurements such as flowrates and temperatures by a Kalman filter by simulation.

(vi) feedforward control of the distillation column using a Kalman filter followed by the comparison of results obtained with those of a conventional control method by simulation.

II.1 THE STATUS OF CHEMICAL PROCESS CONTROL

The status of chemical process control has been the subject of intense controversy in recent years. We are now two decades into the era of modern control theory and many theorists, pointing to the apparent advanced applications in the aerospace industry, wonder at the tardy pace of application in the process industry.

Control practitioners conventionally argue that modern control theory is not relevant to the chemical process control and that classical techniques and designer experience will always lead to satisfactory and perhaps optimal solutions. Publications by these groups have done little to establish a satisfactory dialogue; few practitioners appear to have more than a superficial knowledge of modern control theory; modern control researchers have produced few convincing examples of successful chemical process applications (Wooyoung and Weekman (37)).

Further, the techniques of chemical process control, although superficially in good health, are in many important respects at a point of conceptual stagnation. Even the splendour of digital computers which are now shepherding many chemical processes, cannot hide the pervading thinness of substance in their assigned tasks.

A brief review of the two available control theories for chemical processes, namely the classical and the modern control theories, at this stage, may not go amiss. The outstanding features of the classical

approach are as follows:

(i) a linear model of the system is assumed, and the designer then proceeds to describe the system in terms of transfer functions of either frequency or Laplace variety depending on the type of information available to him

(ii) an almost exclusive emphasis is placed upon specific control systems classified as the servo-mechanisms

(iii) mostly single-input-single-output systems are considered

(iv) it usually draws on the indirect design techniques of the trial-and-error type.

Thus, the classical approach does enjoy the following important and time-tested advantages:

(i) no sophisticated mathematics are required beyond the elements of linear differential equations and complex algebra

(ii) it utilizes a linear model which in the great majority of cases is found to be quite adequate in its representation of the important poles, zeroes and delays at the nominal conditions of opeartion.

Nonetheless, it also suffers from the following disadvantages:

(i) empiricism which may entail lack of generality

(ii) trial-and-error design that may be time consuming

(iii) restriction to single-input-single-output systems only.

Moreover, while acknowledging the usefulness of this classical approach for single-loop systems, some also criticise it for not yielding an optimal control and for its inability to handle non-linearities. These criticisms fade to insignificance when one discovers its total inability to guide the control system design for interacting multivariable processes. The control of both top and bottom compositions of a distillation column is an oft-cited example of control difficulties in interacting chemical processes. While the classical control theory is capable of analysing the difficulty, it has nothing to suggest as a remedy. The seat of its impotence is in its reliance on the designer to specify the control configuration.

The control technique normally employed for chemical plant systems is indeed, much in line with the classical theory inasmuch as it essentially involves choosing a set of measurable variables which when controlled at some value are expected to enforce the quality, throughput and safety requirements of the plant. As far as possible, these variables are then controlled with a collection of single-loop controllers, manipulating easy-to-adjust variables - usually flowrates. Modifications to single-loop concept such as cascade, feedforward, ratio, non-linear elements etc. are then made as they appear necessary. During the start-up of the plant, the mode adjustments in the feedback controllers are adjusted largely by trial and error to achieve adequate performance. Needless to say, this approach draws

heavily on past experience or on pilot-plant control systems.

The single-loop approach has many advantages for the operator, for maintenance personnel and the reliability of the operating unit. It is handily analysed by linear design technique. The rationale of the theory and the methods of application to chemical processes are clearly and succinctly presented by Gould (23). The use of a linear model on inherently non-linear processes is not a restriction of significant consequence in the great majority of cases and this indubitably provides further incentive for the use of this classical technique. Yet another point that can be brought up in favour of single-loop control is the fact that it often facilitates detection of any of a vast number of possible failures in minimum time and hence speedy corrective action becomes possible.

In spite of their many advantages, as stated before, single-loop controls will not always provide adequate control and thus must be improved upon. The most difficult task for the design engineer is to determine first those cases where a simple control system is not sufficient and then to devise an adequate solution using a control system which is as simple as possible.

In view of the inadequacies of single-loop methods in the treatment of dynamically interacting processes, one might be tempted to turn to the theory of non-interacting control (Gould (23)). In this technique a design is sought such that a change in the set point of

one variable affects that variable only. This is achieved by choice of a control matrix such that its product with the process transfer function is diagonal. With diagonalization achieved, the various consequential control loops are then non-interacting and single-loop control theory may be used to design each loop separately. Foss (38), after a review of the shortcomings of this approach, suggests that non-interacting control is not worthy of consideration for process control. According to him, these interactions should be exploited rather than avoided and needless to say exploitation of interaction in multivariable processes "takes brains, judgement and maturity" - not to mention a good theory which remains elusive. Modal control proposed by Rosenbrack (33), is a technique that exploits these interactions to achieve control objectives. This technique will be discussed in more detail at a later stage in this thesis.

The allusion to modal control leads us on to the other approach to chemical process control, namely, modern control theory which encompasses such control techniques as modal control, optimal feedback control, optimal feedforward control, and model reference adaptive control.

It essentially posseses the following features:

(i) it approaches the problem in a more fundamental fashion. For example, it defines the concept of control and establishes test procedures for determining when and under what conditions a system is controllable. Direct synthesis methods

are proposed which lead to unique system designs that are optimal in some defined sense.

(ii) extensive use is made of a computer for analysis of the control problem, synthesis and sometimes for the implementation of the control solutions.

(iii) it does not limit itself to linear models. Therefore, time-domain system descriptions (state-space approach) are preferred to transfer function methods.

(iv) it draws heavily on more advanced mathematics such as calculus of variations and matrix algebra.

Modal control is a novel approach to the analysis and design of control systems for very complex processes. In theory, this method can be used not just to determine the settings of the controllers but also can serve as a systematic guide for selecting control system configuration. The approach is based on the notion that the dynamic behaviour of a system can be represented by the motion of a point in an n-dimensional space (state-space) which leads to a mathematical model in the form of n first order differential equations. The theory essentially centres around the theme that the transient behaviour of a process is predominantly determined by the modes associated with the smallest eigen values. It is, therefore, proposed that the rate of response of these modes be increased to an acceptable level by positioning the mapping of the input control vector in the subspace spanned by the eigen vectors of the controlled system. When this can be accomplished and when

the activation of the modes can be measured, the eigen values or the time constants of the closed loop process can be adjusted independently through a proportional feedback control matrix. In principle very rapid and stable recovery can be achieved. Modal control is thus a technique that exploits interactions among variables to achieve control objectives. However, Foss (38) indicates that, unfortunately, but not unexpectedly, such ideal circumstances do not obtain in chemical process systems. The ability to measure only a very few of the states may lead to inaccurate estimates of modal activations, and the handful of process inputs in general cannot be aligned with process modes. Both these facts of life can, indeed, cause serious deficiencies in control systems designed by the modal techniques. Nevertheless, attempts have been made to apply the idea to the control of diffusive distributed processes, a distillation column, a boiler, and a 41-variable chemical plant model (23, 42, 43). In these investigations knowledge of the modal character of the process was used to suggest the choice of measured and manipulated variables, i.e. the control configuration.

While there remain potentially useful developments of modal control to assist in the determination of control system configuration, Macfarlane (44) points out that there exist several disadvantages to this idea. Primarily, the method gives attention only to the poles of the system; closed-loop zeroes, which could also influence the system behaviour are left unattended.

Further, the method does not address the regulation of specific output variables.

The theory of optimal control, by its very name, would seem to promise a best compromise among all the conflicting requirements of process control systems. But it does not. Rosenbrock and McMorron (109) indicate that "The word optimal carries with it the suggestion that the system has desirable properties in general, but of course, this need not be the case". There are, indeed, many undesirable properties and unworkable features of the theory as it has been developed for chemical processes.

Optimal control, defined in various ways, has been attempted of stirred tank reactors, tubular processes, distillation columns, extraction columns etc. Objectives in these attempts have been to determine (open-loop) manipulatable input histories that minimize the time required to bring the process to a new state or the (closed-loop) feedback and feedforward gains that minimize a quadratic functional of the process states and control inputs. Other objectives such as maximization of reaction yields have also been attempted.

Upper and lower bounds on the control input are imposed in the time-optimal case with the result that the optimal inputs may reside at one or the other bound for all or part of time (so-called bang-bang control). The switch from one bound to another is determined by switching curves that are calculated from the necessary conditions for minimum time, a calculation involving the integration of the state and adjoint differential

equations with split boundary conditions. The calculations are difficult and lengthy. In all this, of course, one assumes perfect knowledge of the process model and parameters and that there are no process disturbances.

Foss (38) goes on to say that in view of the unlikely attainment of these assumptions and the infrequency of purposeful state changes, startups and shutdowns in continuous processes, it is difficult to appreciate the utility of such a theory for the control of chemical processes.

Various attempts have been made to develop algorithms for the computation of this type of control which can be very difficult to understand. Perhaps the usefulness of such a theory can be argued in some special cases but, in the light of the circumstances encountered in chemical processes, its quantitative value is slim for the processes and situations so far treated in the chemical engineering literature.

Optimal feedback control, viewed with respect to applications to chemical processes treated so far appears to be no less immune from criticism. A review of the reasons as to why optimal feedback control is also open to such powerful criticisms has been given in the aforementioned paper by Foss.

Therefore, it appears rational to finish by saying that investigation into requirements for good process control is imperative. It has been argued here that problems, needs and objectives of process control differ so significantly from those in other fields that

the nearly direct translations of methods developed elsewhere have little practical values for process control. We must always remember that our systems are nonlinear, usually slow-moving, contain appreciable dead times and are subject to unknown disturbances. These problems are further compounded by the fact that our mathematical models are usually inaccurate, the system parameters are normally uncertain and primary process variables are very often difficult to measure.

II.2 CONTROL OF DISTILLATION COLUMNS : THE LITERATURE REVIEW

The literature abounds with applications of various methods for control of distillation columns. The objective here is to review these methods and, where need be, concisely expound their theoretical concepts in an effort to explain how they relate to the classifications introduced in Chapter I. Attempt is also made to highlight the relevance and the possible use of an estimator in relation to those methods where appropriate. The model-independent feedback methods essentially constitute the deductive approach while the model-dependent methods such as feedforward and modal form the mathematical path to the control of distillation columns.

II.2.1 THE DEDUCTIVE APPROACH : MODEL-INDEPENDENT FEEDBACK CONTROL METHODS

Model-independent feedback forms of control have been the traditional methods of controlling distillation columns and have often provided acceptable control despite scant knowledge of the dynamic character of the column. The deductive path, referred to in Chapter I, is essentially constituted by the feedback forms of control in which attempts are usually made to reduce interaction in the column without recourse to a mathematical model and using conventional hardware. At the risk of being tautological, one must restate that the guidelines followed in the deductive path have been past experience, inference and empirical structures and, indeed, this fact is echoed in the forms of control that will be discussed in this section. In control language, the deductive path differs from the mathematical path in two different ways. Primarily it avoids the problem of the dynamicsand secondly, the synthesis stage is normally accomplished by single-input-single-output (SISO) methods or, more often by on-line tuning.

The following forms of control that have appeared in the literature are basically deductive:

(i) single-plate temperature control

(ii) multiple-plate temperature control

(iii) material balance control

II.2.1-1 Single-Plate Temperature Control

On-line control of distillation columns requires that a measurement should be made of the composition of the product or of some variable which is indicative of the product composition. The most common measurement used for product quality control is a tray temperature near the end of the column from which the product comes. The location of the tray for temperature measurement is very important. It should ideally be at a tray which exhibits a reasonable temperature variation when product quality changes, yet be near the end of the column producing the product whose purity is being controlled. A large number of workers have suggested that product quality should be controlled at both ends, yet a lot of columns are still solely controlled at one end. This is by virtue of the effectiveness of separation in one half of a column which negates the necessity for control loop in that half owing to the over design of the columns. Therefore, single-plate temperature control simply means a control based on a single temperature measurement in either the enriching or the stripping sections.

The most usual single-plate temperature control scheme is depicted in Figure II.2.1. Here, the reflux drum and reboiler levels are controlled by the product off-take rates. The product quality at either end - as assessed by the temperature measurements near the ends of the column - is controlled by the amount of recycle to each end of the column.

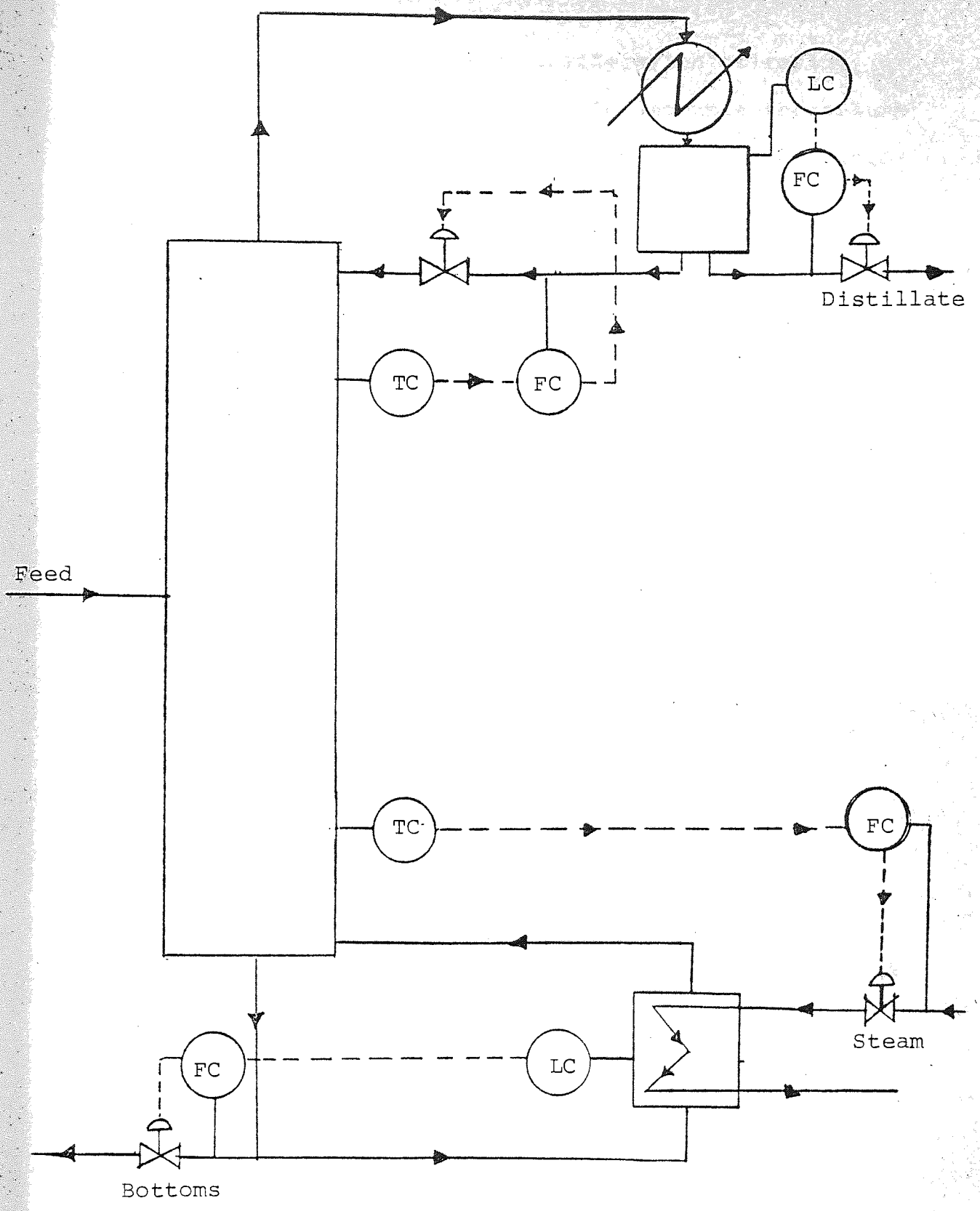


Figure II.2.1. The Standard Control Scheme for Distillation Columns.

Based on McCabe-Thiele consideration of reflux ratio and in an attempt to start to decouple the column, some workers (45,46) have introduced the idea of ratio-ratio control. In this approach, the hold-up tank levels are controlled by the product off-take rates and the ratio between the recycle rate and the product off-take rate at either end is controlled by a temperature measurement near the ends of the column.

Jordan (25) points out that it is of paramount importance to note that these methods satisfy the steady state requirements of the column but not necessarily the dynamic requirements of the control system. Moreover, the attempt to decouple a physical system appears to be unrealistic.

These workers have also suggested that for more accuracy, measurement of pressure near the temperature measurement point is requisite. Normally, a simple temperature measurement of the boiling point is used to assess the composition but in presence of pressure variations this practice becomes inaccurate. Therefore, the pressure in conjunction with temperature may give a better approximation to the composition on the plate. The schematic diagram of a ratio-ratio control structure using pressure-corrected temperatures is given in Figure II.2.2.

It is suggested that ratio-ratio control can readily cope with situations where levels initially change faster than temperatures.

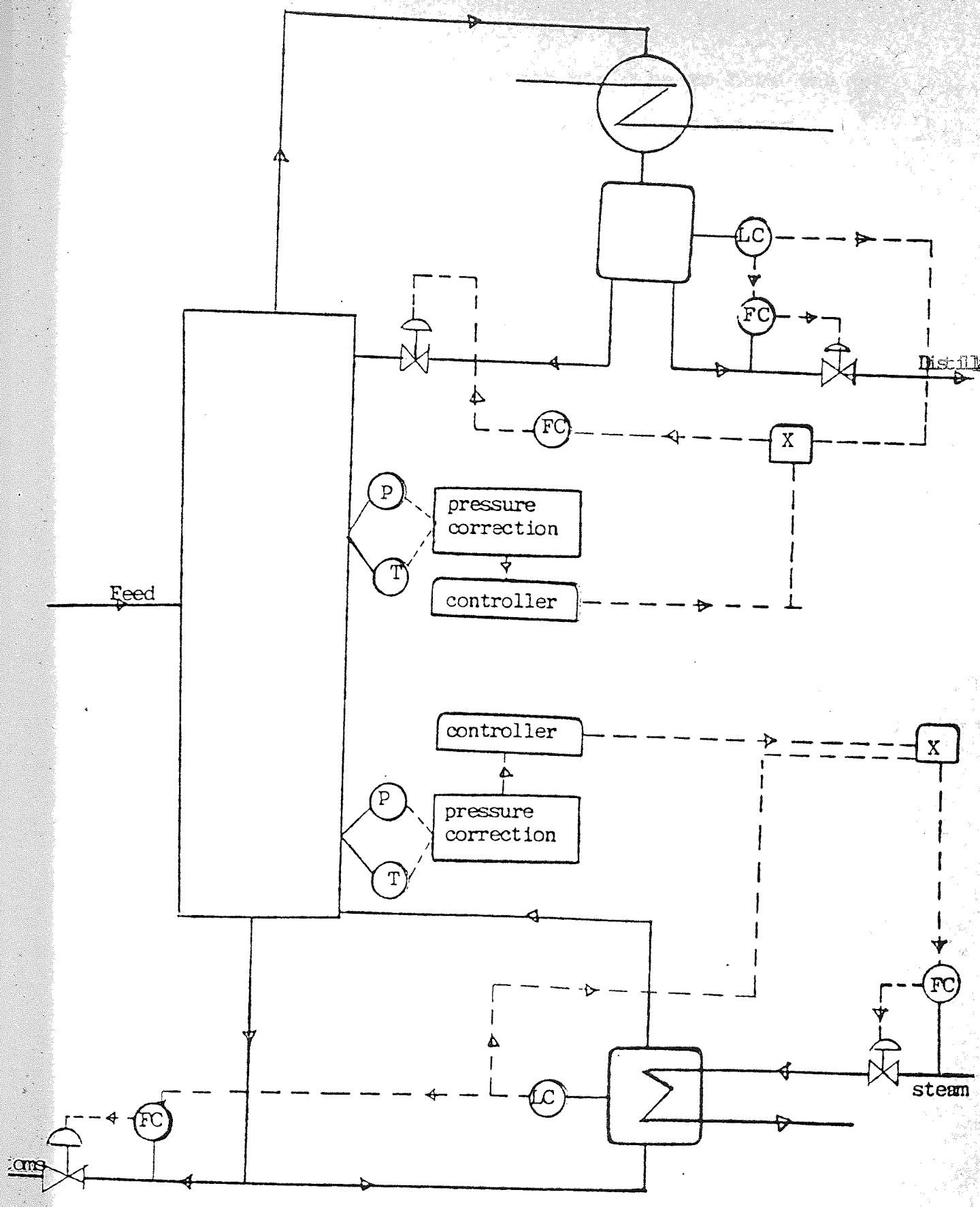


Figure II.2.2
The control structure for ratio/ratio control using pressure corrected temperatures

Another possible structure would be to have the levels control the product rates while the bottom temperature trims the ratio between the reflux and the steam rate as illustrated in Figure II.2.3.
This control structure is problematical owing to the fact that the trimming of the control loop is highly critical. If the bottoms level starts to drop due to a reduction in the feed rate, the bottom level controller will reduce the bottoms rate and due to the ratio between steam and the bottoms rate, the steam rate drops off, and this, in turn, leads to a reduction in the reflux rate due to the second ratio unit. The reduction in the reflux rate means a lower liquid rate into the bottom holdup and, therefore, this leads to a further cutback in the bottoms rate. In other words the system is undesirably at minimum phase. Comparative results using this kind of structure to control a column subject to feed changes have been unimpressive.

A variety of such schemes have been proposed by Perry (1), Gould (23) and Shinskey (18) to deal with various situations encountered in practice.

Rosenbrock (47) suggests that interaction can be further reduced by controlling (x_1+x_2) with the reflux and (x_1-x_2) with the reboil : x_1 and x_2 stand for the composition measurements at either end which are normally inferred from temperature measurements.

It is of interest to note that Rosenbrock's proposal is embodied in an appendix to his paper and in fact, later in the same year, he propounded the notion of

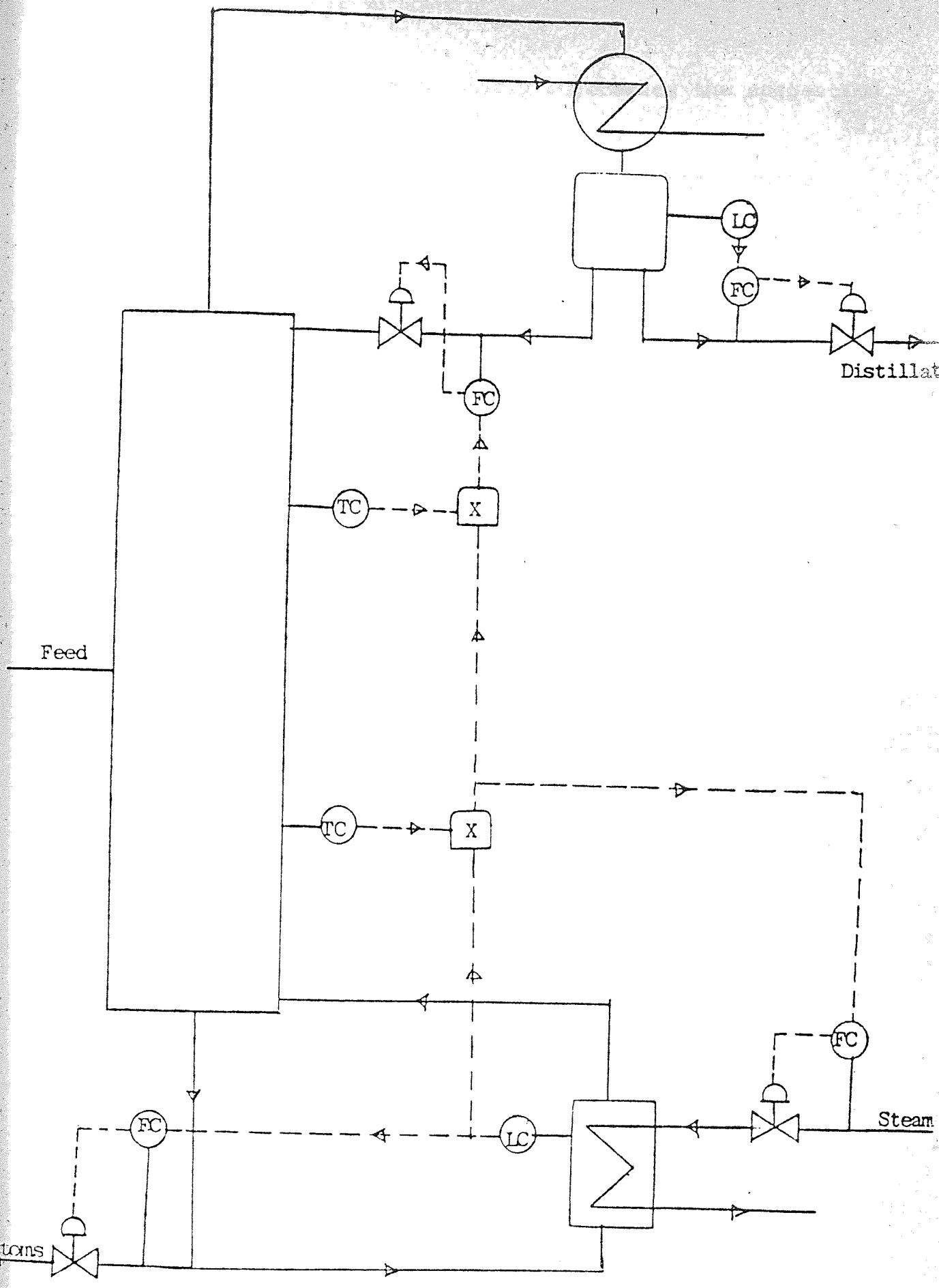


Figure II.2.3
A control structure which attempts to allow for internal interaction between reboil and reflux.

modal control which effectively supersedes the suggestion mentioned above.

It goes without saying that in all these control exercises, the proper tray location for temperature measurement is of utmost importance. The proper tray can often be determined by measuring the temperature profile of the column experimentally. A typical distillation column temperature profile is depicted in Figure II.2.4.

II.2.1-2 Multiple-Plate Temperature Control

In an attempt to improve control, some authors (45, 46) have suggested pressure corrected temperature measurements while others have proposed the use of several temperature readings.

As an example, one could, at the outset, mention the work of Weber (48) who measured the temperature difference between two points in a section of the column to control it. The sole advantage of this approach is reflected in the fact that both temperatures are affected by pressure changes in the column and because the difference is used, the effect of pressure on the boiling point can be neglected.

Luybon (49) used a double-differential temperature as the input to the controller. This is best elucidated in Figure II.2.5. Here the controller input is $(B_2-B_1) - (B_3-B_2)$ or $2B_2 - (B_1+B_3)$ where:

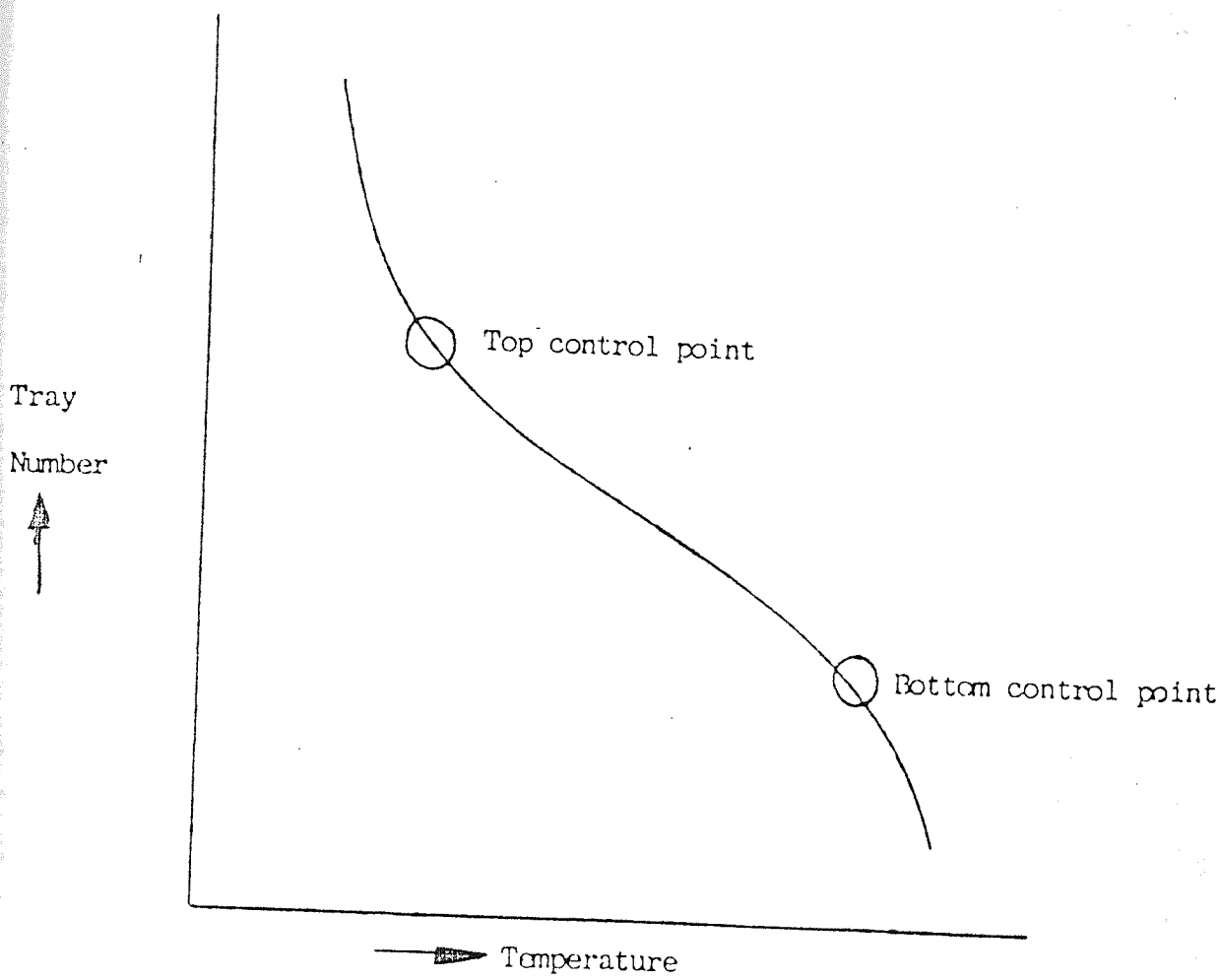


Figure II.2.4. Column temperature profile with typical temperature-control-measurement location for binary mixtures

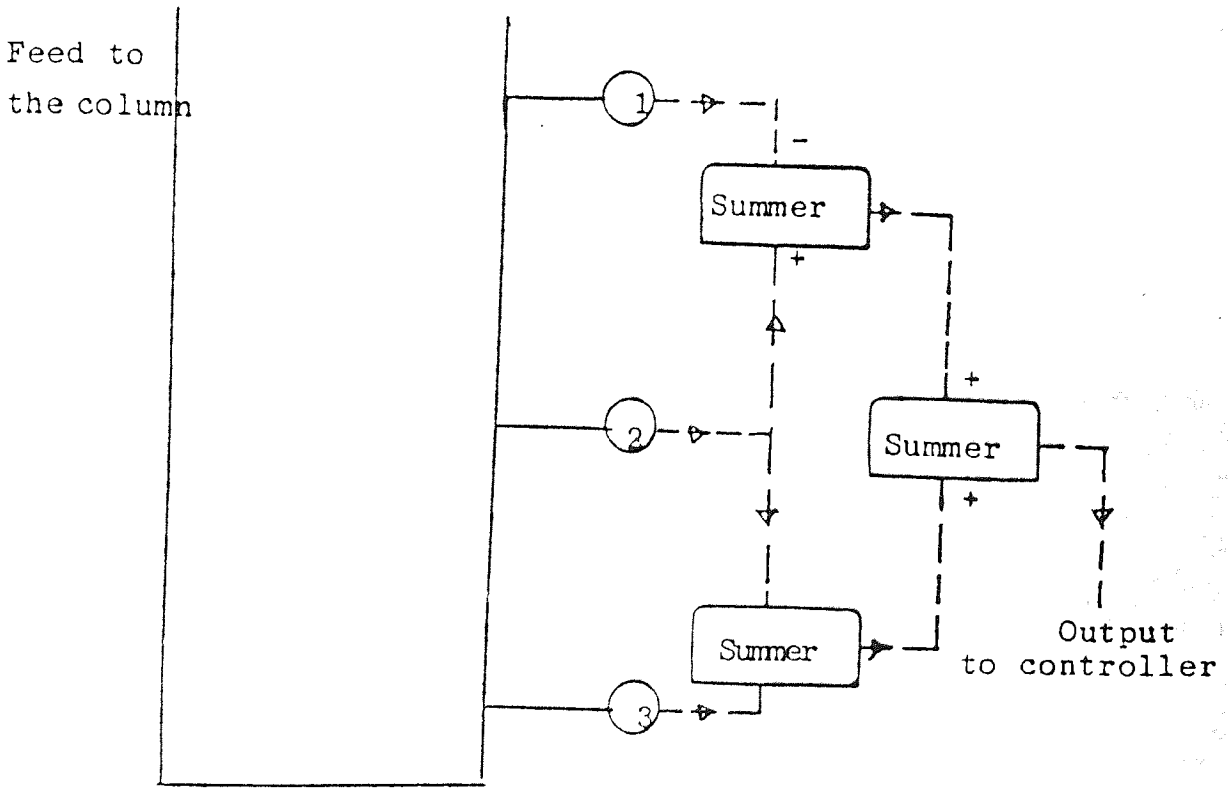


Figure II.2.5

The hardware for the implementation of Luyben's double differential temperature control scheme

B_1 = temperature measurement near the feed plate

B_2 = an intermediate temperature

B_3 = bottoms temperature

Luyben states that this scheme gives a better steady-state control than pressure-corrected temperature. However, he also states that dynamically the ameliorations obtained using this scheme are not significant.

Aside from the multiple-plate and pressure-corrected temperature methods, which can be regarded as being relatively minor variations of the single-plate temperature control scheme, there has not been any progress in furthering the effectiveness of this comparatively simple, but useful technique.

II.2.1-3 Material Balance Control

The material balance control scheme introduced by Shinskey (52), is essentially based on steady-state overall and component balances over the column which for a binary system would lead to the following control equation

$$D = F\,\frac{z-x}{y-x} \quad \text{or} \quad B = F\,\frac{y-z}{y-x} \qquad \text{..... II.2.1}$$

where

F,D and B are the feed, distillate and bottoms rates respectively.

z,x and y are the feed, liquid and vapour compositions of the most volatile component

Additionally, for two-point control, the separation factor is defined as:

$$S = \frac{y(1-x)}{x(1-y)} \quad \text{..... II.2.2}$$

It is throught that if separation is held constant, the control of y will also result in control of x and vice versa.

Four possibilities for the manipulated variables have been suggested namely:
D,B, boil-up rate V, and reflux rate L. In a later paper (1975) Shinskey (32) introduces heuristics for pairing these variables in order to reduce interaction between them. These are as follows:

(i) when only one product quality is to be controlled then the material balance should be manipulated

(ii) the lesser of the two products should be manipulated for product control

(iii) the material balance should be manipulated to control the quality of the less pure product and the separation factor should be manipulated to control the quality of the more pure product

The authors indicate that enforcing control over the external material balance alone does not ensure the control of product quality. Compositions are determined by the relative flows of vapour and liquid within the column, so these are the streams which ultimately must be regulated. To bring this about, it has been emphasised that automatic level control, say on the reflux drum is imperative. It is also of interest to

note that Shinskey (52) advocates the use of level-controllers to manipulate the reflux flow. There exists a general reluctance in using such arrangements. This is due to the fact that valve-moter hysteresis can lead to a degradation in the liquid level control and this in conjunction with the integrating characteristics of the accumulator could cause intolerable limit cycle (53). Despite these likely problems, it is thought that the arrangement is stable and is being used successfully.

Fauth and Shinskey (20) implemented material balance control on a depropanizer column and, according to them, the results were staggeringly successful so far as the economic impact of the operation was concerned. They also studied local optimization, and floating pressure control and showed that these techniques could also pay off in terms of profitability and reliability.

Gaulier and McCune (54), working on the idea that internal reflux flow within a distillation column can rarely be the same as the external reflux flow, incorporated an internal reflux controller into the conventional material balance scheme. They used the equation suggested by Lupper and Berger (55) which relates the internal and external reflux flows and is as follows:

$$R_I = R\{1 + (C_p/\lambda)(T_o - T_r)\} \quad \text{..... II.2.3}$$

where

R_I = internal reflux flow

R = external reflux flow

T_o = overhead vapour temperature

T_r = the reflux liquid temperature entering the column

C_p = molar specific heat capacity between T_o and T_r

λ = latent heat of vaporization at T_o

According to the aforementioned article, they managed to get almost perfect compensation to condenser duty changes. The degree of compensation depended upon how tightly the overhead level had been controlled. The major criticism that may be directed towards their work is the fact that they ignored such limiting factors as flow and level measurement noise.

It must be pointed out that while material balance control is applicable to binary distillation columns, it is virtually impossible to see how the principles could be extended to a multicomponent distillation situation.

II.2.2 THE MATHEMATICAL PATH : MODEL-DEPENDENT METHODS

By contrast with the deductive path where the synthesis stage is usually accomplished by the single-input-single-output (SISO) design methods, the mathematical path is characterised by the fact that the synthesis stage is normally carried out by the multivariable design methods. The difference is that the multivariable design methods take interaction into account whereas the SISO methods do not.

II.2.2-1 Non-Optimal Model-Dependent Feedback Methods

Little has hitherto appeared in the literature concerning the non-optimal model-dependent feedback control methods for distillation columns. The use of a model in conjunction with the feedback philosophy has been, in fact, mainly advanced by the need for the proper tray location for temperature measurement. The role of the model has essentially been to assist in finding the proper tray for temperature measurement instead of measuring the temperature profile of the column experimentally as in the deductive path.

Proper tray location by tray-to-tray calculation has been investigated by various workers who have proposed different mathematical models for predicting the dynamic response of the column with different control plate locations. In many cases, the models have been developed from data for open-loop transients which are dominated by the large major time constants

of the column and often show strong non-linear effects (Moczek and Williams (56)). To account for the changes in response time with plate location and type and magnitude of the disturbances, the models must be quite complex and are not convenient for control studies. However, for simulation of closed-loop control systems where deviations from set-points are generally small and the non-linearities are relatively unimportant, simpler models may be satisfactory.

An approximate model based on a linear analysis is presented by Wahl and Harriot (57) which can be used to predict typical column transfer functions and the effect of control plate on critical frequency, maximum controller gain and steady state error in product composition. More recently, this model was tested experimentally by Beaverstock and Harriot (58), who measured the closed-loop response of a column for various plate locations. The conclusions that they reached may be summarised as follows:

(i) for control of the top product composition by feedback manipulation of the reflux rate, moving the control point down the column decreases the critical frequency and the maximum controller gain because of increasing the number of hydraulic lags, and also increases the steady-state error in product composition. These effects suggest that the control plate should be as close to the top as possible, consistent with measurement accuracy.

(ii) when the measurement and valve lags are small, two-mode feedback control can correct for moderate (10-20%) changes in the feed rate and feed composition with barely noticeable changes in product compositions. Similar changes in vapour flow produce greater upsets, partly because vapour changes are transmitted rapidly through the column and partly because of the effect of vapour flow on plate hold-up.

(iii) a linear model seems satisfactory for predicting the effect of control plate location and for comparing control schemes. However, they state that more work is required to predict the hydraulic lags and the effect of vapour rate changes.

II.2.2-2 Feedforward Control

In application of feedback control to distillation columns corrective action is taken only after the product qualities have deviated from their desired values, and long times are often required to bring the column to its desired steady state - especially in large towers. Also, undesirable interaction of feedback loops may occur as most columns are multivariable.

Feedforward control in principle eliminates these difficulties by sensing the input disturbances as they enter the column and taking proper corrective action before these disturbances have propagated through the system. Thus control problems inherent in dead time

and distributed parameter systems are theoretically eliminated. However, feedforward control in practice has its limitations. First, the system may not correspond exactly to the mathematical or empirical model used to predict its dynamic behaviour. Second, changes in product compositions caused by unmeasured input disturbances may go uncorrected.

The literature on application of feedforward control to distillation columns is far from voluminous. Luyben and Gerster (59) suggest a transfer function between the input disturbances (feed rate, F, and feed composition, Z_f) and the manipulative or corrective inputs (reflux rate, R, and vapour boil-up rate, V) such that the control objectives, that the perturbations in the compositions of the overhead and bottoms products be zero, are met. The feedforward controller of their distillation system, assuming it to be linear, was made up of four separate transfer functions; in matrix notation these were:

$$FFC = \begin{bmatrix} R/F & R/Z_f \\ V/F & V/Z_f \end{bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{II.2.4}$$

Therefore, if the transfer functions are known and if upsets in feed rate and feed composition are measured, the proper values of the corrective inputs are readily determined accordingly to:

$$\begin{bmatrix} \delta R \\ \delta V \end{bmatrix} = \begin{bmatrix} R/F & R/Z_f \\ V/F & V/Z_f \end{bmatrix} \begin{bmatrix} \delta F_m \\ \delta Z_{fm} \end{bmatrix} = \left| \text{FFC} \right| \begin{bmatrix} \delta F_m \\ \delta Z_{fm} \end{bmatrix} \quad \text{.. II.2.5}$$

where

F and Z_f are the feed rate and composition at steady state

δF_m and δZ_{fm} are the measured upsets in F and Z_f

R and V are the reflux and boil-up rates at steady state

δR and δV are the corrective inputs

FFC = feedforward transfer function

The transfer functions were determined by solving the system's equations in the frequency domin by the stepping technique - the details of which are explained by Luyben (3).

Their experimental results are indicative of the immense potential of feedforward control for distillation columns. Despite the changes in feed rate and feed composition, the product compositions did not change appreciably and there was no detectable transient period.

Another practical limitation of feedforward control stems from the fact that physical and process limitations such as maximum valve opening may constrain the action required by feedforward control. Under such circumstances, in order to prevent drifts of the product compositions, combined feedforward-feedback controls have been suggested. Little attention has

been given to the problem of combining feedforward with a feedback control system. Lupfer and Johnson (61), Luyben (60) and Shinskey (17) have, however, discussed these concepts qualitatively.

Luyben (62) studied the use of feedforward control on a distillation with feedback control of intermediate control tray temperatures. This effectively meant that the feedback controllers did not control the product compositions directly. The feedforward controller which conventionally changes the manipulative variables, had the additional task of adjusting the feedback controller setpoints. It is interesting to note that they have stated that the addition of feedforward control reduced the feedback interaction.

Ballinger and Lamb (63) produced a theoretical analysis for the combined feedforward-feedback control systems which was implemented by Godman and his colleagues (64) to control a column simulation. It appears that the benefits of feedforward control used additionally to feedback control is largely dependent upon the steady-state effectiveness of the feedforward control system.

The likely drawbacks of feedforward control are due to model inaccuracy and the fact that unmeasured disturbances can go uncorrected. This is where an estimator can play an effective role since it should be capable of eliminating these problems to a large extent.

II.2.2-3 Modal Analysis and Control

Modal analysis, introduced by Rosenbrock (33) can, in theory, be used not just to determine controller settings but also can serve as a systematic guide for selecting the control system structure or configuration - i.e. for pairing controlled and manipulated variables. The approach is based on the idea that the dynamic behaviour of a system can be represented by the motion of a point in an n-dimensional space called state-space which leads to a mathematical model in the form of n-first order differential equations. In this picture the central theme is that the transient behaviour of a process is predominantly determined by the modes associated with the smallest eigenvalues. If it is possible to approximate a high-order system by a lower-order system whose slow modes are the same as those of the original system, then attention can be focussed on the attempt to alter the eigenvalues of the slow modes so as to increase the speed of recovery of the process from disturbances. Obviously, various disturbances excite the modes differently so that a scheme which is based on a lower-order model may be inappropriate if a disturbance injects most of its "energy" in a fast mode which has been neglected. However, implicit in Rosenbrock's approach is the possibility of altering each mode separately so that the resulting control system can be viewed as being non-interacting in the sense that manipulation of one mode may not alter any other mode. Thus, it may be possible with enough

measurements and controls or manipulations to speed up the recovery from any expected disturbance. There are obvious limitations to this, since not all the states can be measured in practice and controls cannot be applied to all the states. This will limit the extent to which the speed of recovery of a mode can be increased.

Modal control can, therefore, be defined as a control that changes the modes of a system to achieve control objectives. In other words, a control scheme in which the manipulated variables are operated in such a way that their action is along the eigenvectors of the uncontrolled system. A brief demonstration of the mathematics associated with modal analysis and control, at this stage, would be in order. These appear more fully in Rosenbrock's original paper and in a more recent paper by Simon and Mitter (66).

It is assumed that the linearised equation of the uncontrolled system, in matrix notation, is:

$$\dot{\underline{X}} = \underline{A}\,\underline{X} \quad \text{..... II.2.6}$$

where

$\underline{X}$ = vector of state errors

$\underline{A}$ = relating matrix (nxn)

Supposing that all the natural frequencies (eigenvalues) of the system are real, negative and distinct, then to every eigenvalue of $\underline{A}$, λ_i will correspond an eigen vector $\underline{V}_i$ which represents one of the modes of the system.

The aim is to reduce $\underline{X}$ to the zero vector with utmost speed. A possible solution of equation (II.2.6) is:

$$\underline{X}_i = \alpha_i \underline{V}_i \exp(\lambda_i t) \quad \text{..... II.2.7}$$

i.e. a disturbance in the system grows according to $\alpha_i \underline{V}_i \exp(\lambda_i t)$ along each eigenvector with α_i being a constant. Assume that the eigenvalues of $\underline{A}$, λ_i are real, negative and distinct and that

$$\lambda_n < \lambda_{n-1} \text{ ..... } < \lambda_2 < \lambda_1 < 0 \text{ ..... II.2.8}$$

We aim to shift as many as possible of these eigenvalues to greater negativity; so if there are p manipulatable states, we aim to make $\lambda_1, \lambda_2, \ldots \lambda_p$ as negative as possible.

If we write $\underline{C}$ as an (nxp) matrix having as its columns $\underline{V}_1, \underline{V}_2, \ldots \underline{V}_p$ and $\underline{B}$ as an (nxp) matrix having as its columns the eigenvectors of $\underline{A}^T$ corresponding to $\lambda_1, \lambda_2, \ldots \lambda_p$, the following feedback system can be adopted:

$$\dot{\underline{X}} = (\underline{A} + \underline{C}\underline{K}\underline{B}^T)\underline{X} \quad \text{..... II.2.9}$$

Where $\underline{K}$ is a diagonal (p,p) matrix with non-zero elements $-K_1 \ldots -K_p$. The eigenvalues of this system are now $(\lambda_1 - K_1)$, $(\lambda_2 - K_2)$, ... $(\lambda_p - K_p)$. Therefore, by using large negative values of $K_1, K_2, \ldots K_p$, the rate of decay of disturbance can be accelerated.

$\underline{C}$ is in fact the matrix of vectors along which the measurement vector $\underline{B}^T\underline{X}$ should be forced to move. $\underline{K}$ thus

becomes the matrix of proportional feedback gains acting on the vector $\underline{B}^T\underline{X}$.

Searson (45) found that the dynamics of the modal system compared favourably with the conventional two-term controller systems. For good response, however, elements of $\underline{K}$ still needed to be tuned.

In the application of modal control to distillation columns, it would appear that one should use many measurements in the state vector; this is not the case because modal control aims to reduce the vector to zero and should the composition profile in the column change, this goal will evidently be impossible to achieve.

Introduction of integral action into the feedback controllers would probably improve the steady-state of the system. But introducing further terms into the controller would mean that more controller gains would have to be tuned. However, decoupling the system should enable the feedback loops to be tuned more rapidly and efficiently - owing to their greater independence of each other.

A modal controller has been proposed by Davidson (40) which uses a feedback from:

(i) a temperature measurement near the top of the column

(ii) a temperature measurement near the bottom of the column

and (iii) the pressure at the top of the colum

to control:

(i) the reboiler steam temperature

(ii) the condenser cooling water temperature

(iii) the top product offtake rate

The author states that the results obtained using this controller are significantly better than those obtained from the more conventional schemes. The criterion used for comparison was the reduction of errors in the products due to changes in the feed composition, the reflux and the condenser temperatures. It must be indicated that his results were obtained on a simulation of an 8-plate column and the changes simulated bear little resemblance to the ones experienced in practice. It is also worth noting that Davidson states that a pressure correction to a measured temperature provides a significant drop in the interaction encountered.

It would be interesting to find out how a modal controller would perform in the presence of an estimator which can be used to estimate the states that cannot be measured. The literature contains no evidence of such attempts to apply modal control plus a filter to distillation columns.

II.2.2-4 Optimal Control

Detailed discussion of the optimal control problem and the methods of solution available up to date would be too voluminous to incorporate into this thesis and, also, it exceeds the scope of this thesis. Nonetheless, for completeness, suffice it to make an attempt

to introduce, succinctly, the problem and to review, briefly, the methods that may be adopted to solve the problem whether they be analytical or numerical. These appear more fully in a book by Prime (66).

To date, little has appeared in the literature concerning the optimal control of distillation columns. However, a fairly comprehensive review of the work done in the field is given by Jordan (25) while Walter (26) presents a closed form analytical solution to the problem.

II.2.2-4.1 Statement of the Optimal Control Problem

Consider a linear plant which obeys the matrix equation:

$$\dot{\underline{X}}(t) = \underline{P}\underline{X}(t) + \underline{D}\underline{U}(t) \quad \text{..... II.2.10}$$

where

$\underline{X}(t)$ = the state vector

$\underline{P}$ = the plant matrix

$\underline{D}$ = the driving matrix

$\underline{U}(t)$ = the control effort vector

The general objective is to determine the control vector $\underline{U}opt$ which minimises a performance criterion, J. J is, usually, a quantitative scalar cost function that enables comparisons between systems to be made. A common cost function is Lagrangian of the type:

$$J = \text{Min} \int_0^T L(x_1, x_2 \ldots\ldots x_n;\ U_1, U_2 \ldots\ldots U_n).dt \quad \text{.. II.2.11}$$

II.2.2-4.2 Solutions of the Optimal Control Problem

(a) The analytical Solutions

Much of the work done in this field has been inspired by the contributions of Kalman (68) who introduced the matrix-Riccatti equation as a means of solution. The analytical solutions of the optimal control problem can be broadly categorised into two classes:

(i) solutions by variational calculus

(ii) solutions by dynamic programming

Solution by variational calculus involves treating the problem as a minimization problem in variational calculus where the performance criterion equation is to be minimised subject to the constraint equation:

$$\dot{\underline{X}}(t) - \underline{P}\,\underline{X}(t) - \underline{D}\,\underline{U}(t) = 0 \quad \text{..... II.2.13}$$

Thus, having defined the complete set of Pontryargin equations, one then proceeds to derive the matrix-Riccatti equation and hence an optimal feedback controller. Closed form solutions of the matrix-Riccatti equation are investigated by Walter (26) and Jordan (25).

Brosilow and Handley (67) implemented optimal control on a 15-plate, five inch diameter bubble cap column and measured the temperature on every plate : these temperatures were used as the elements of the state vector. The started from:

(i) a linear plant equation

$$\dot{\underline{X}} = \underline{A}\,\underline{X} + \underline{B}\,\underline{U} \quad \text{..... II.2.14}$$

(ii) integral squared error criterion

$$J = \text{Min} \int_{o}^{\infty} \{\underline{X}^T \underline{Q}\, \underline{X} + U^T R\, U\}.dt \quad \ldots\ldots\ \text{II.2.15}$$

(iii) the matrix Ricatti equation

$$\underline{P}\,\underline{A} + \underline{A}^T\underline{P} - \underline{P}\,\underline{B}\,\underline{R}^{-1}\underline{B}^T\underline{P} = -\underline{Q} \quad \ldots\ldots\ \text{II.2.16}$$

where

$\underline{X}$ = state vector (nxl)

$\underline{A}$ = process matrix (nxn)

$\underline{B}$ = matrix of process constants (nxm)

$\underline{P}$ = Ricatti matrix (nxn)

$\underline{Q}$ = positive semi definite weighting matrix (nxn)

$\underline{R}$ = weighting matrix (mxm)

$\underline{U}$ = input, vector (mxm)

They assumed $\underline{R} = \underline{O}$ in order to achieve an approximate solution.

An unfortunate side-effect of this formulation is that a steady-state offset is produced by a feed composition change because the policy attempts to maintain the weighed vector of state at zero. Brosilow and Handley produced no comparative results to show how their optimal control policy fared in competition with conventional controllers.

Williams (69), in his report, on various control techniques for distillation columns concludes that optimising a control scheme by a dynamic programming method is far too complex. He was attempting to control the top product composition by maintaining a steady boil-up rate. Dynamic programming gave results

similar to those obtained by other ocntrol structures. The complexity of dynamic programming is, of course, approximately proportional to the square of the number of states used. Thus Williams' conclusion that dynamic programming is too complex would seem to be damning. He mentions minimising a quadratic performance index but does not discuss its implementation. But it is significant that he finally concludes that model-based control systems provide better controllers than systems tuned on-line and that control systems using second-order models are indistinguishable from those using first-order models.

Lapidus and Luus (70) have presented an algorithm for the solution of the optimal control problems for a non-linear system. This algorithm is a clear indication of the excessive amount of calculations required for solving the optimal control problem.

An obvious use for an estimator in relation to optimal control would be to use it to estimate the states that cannot be measured.

II.2.2-5 Adaptive Control

During the last decade adaptive control has often been forecast to become a common development of control systems in the chemical process industries. In this approach one essentially tries to compensate for the process parameter variations. For instance, in conventional PID controller,

the parameters K_C, T_I and T_D are updated as the information about the process becomes available. Figure II.2.6 shows a schematic diagram illustrating a possible way of implementation of adaptive control.

Many different types of adaptive control algorithms have appeared in the literature mostly concerning the SISO systems. But few successful applications have been reported, especially as regards distillation columns. In fact the only traceable example to date is due to Van Aarle (71) who studied the adaptive control of a high-vacum distillation column. He concludes that unless the variations in process parameters are known to hamper control, this type of extensive analysis is difficult to justify. Van Aarle was mainly concerned with plant-adaptive control and identified the following functions that should be performed by an adaptive controller:

(i) identification : deriving information about the process parameters from the observable variables of the process. At this stage, two concepts can be distinguished.

  (a) plant-variables adaptive control, where changes in process transfer function are predicted from measurements of the relevant plant variables with the aid of a pre-established relation (e.g. between a dead time and equipment throughput)

  (b) plant-characteristic adaptive control, where the process transfer function is estimated

from measurements of the process inputs and outputs possibly with the aid of the psuedo-random binary sequence (PRBS) technique

(ii) decision : deciding to change the control scheme if the present performance is estimated to be too far below the optimal performance

(iii) modification : adapting the structure or the parameters of the control system

In contrast with the plant-adaptive control concept, an alternative approach is the model-reference adaptive control which is depicted in Figure II.2.7. Here the response of the model is checked against the real system's response and the difference is used to modify the model and, or, the controller parameters. Takahashi (24) points out the two important examples of such systems, namely the dynamic observer (72) which is used for estimating the state of the system for which the initial state is unknown, and the Kalman filter (73), which is used for state and parameter estimation of a system in a noisy environment.

Multivariable aspects of adaptive control has been briefly discussed by McConcell and Swanick (74) while Price (75) discusses yet another adaptive control technique known as the accelerated gradient method. This is essentially based upon the objective of improving the stability characteristics of model reference adaptive control and can be useful for slowly moving parameters.

It is significant to note that all of the model reference adaptive control methods exploit the principles of feedback.

Figure II.2.6 : A Typical Adaptive Control Scheme

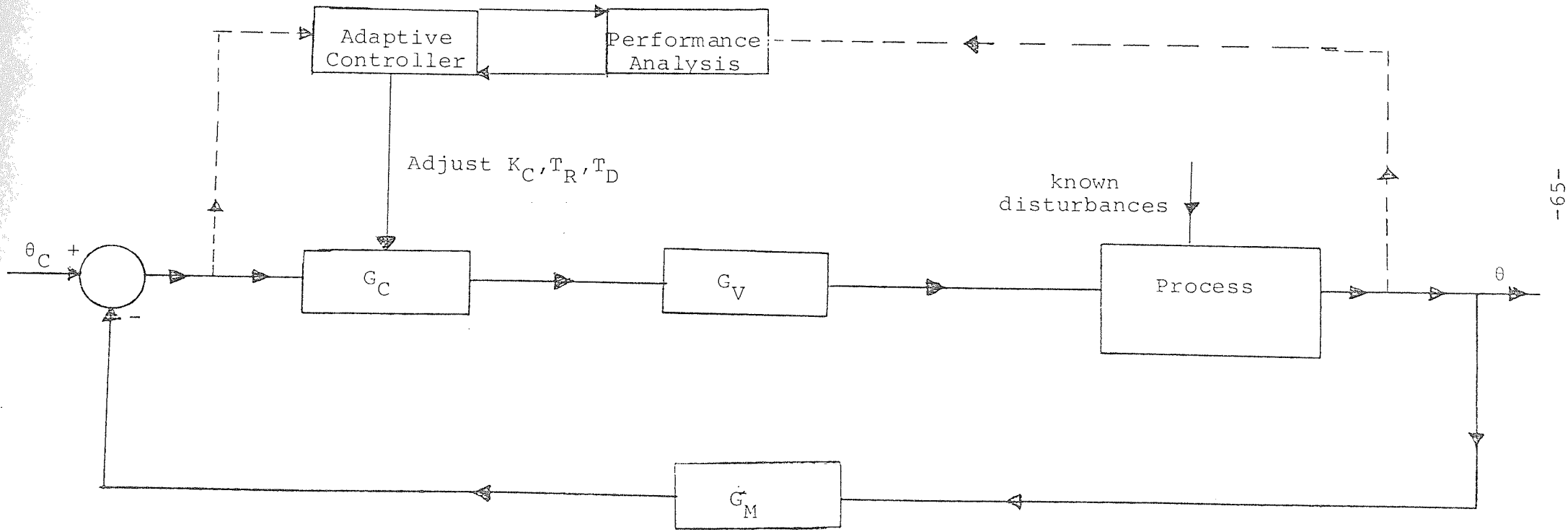
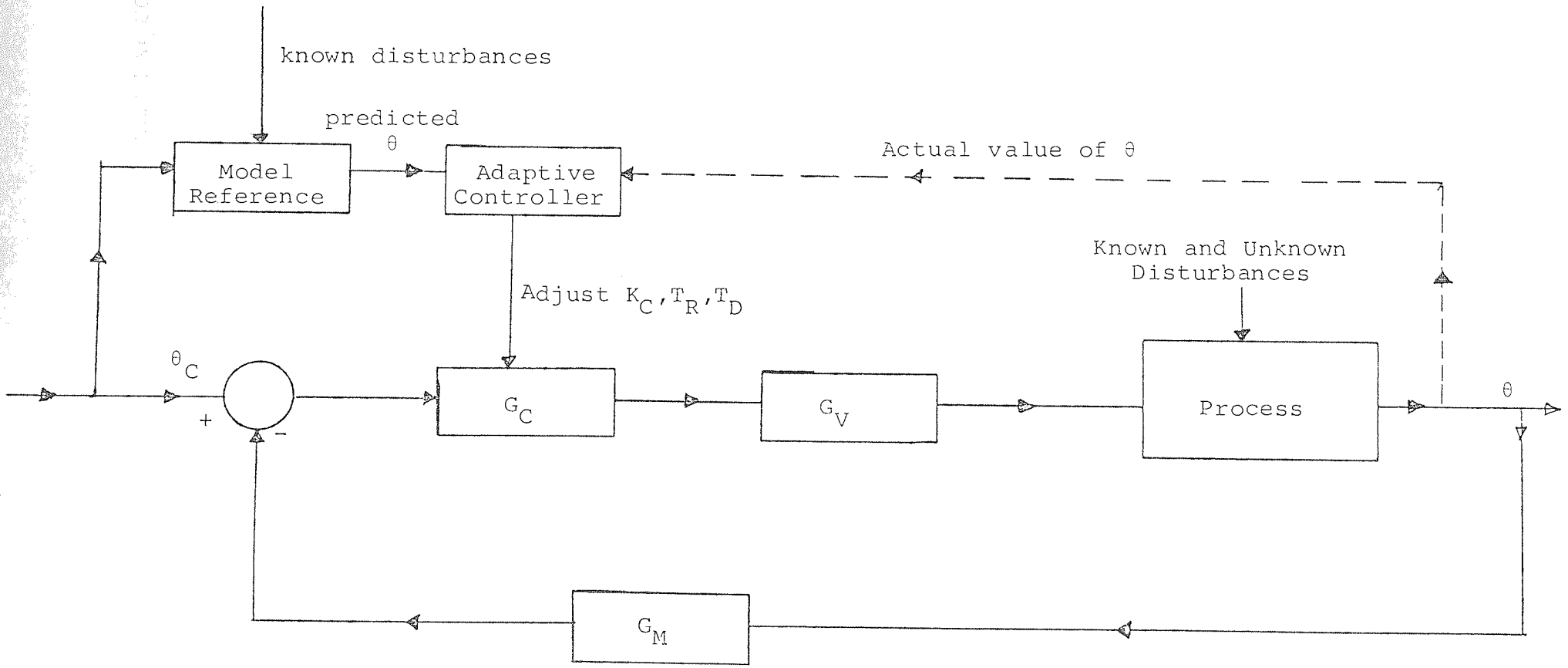


Figure II.2.7 : Proposed Model Reference Adaptive Control Scheme



II.3 DYNAMIC SIMULATION OF DISTILLATION COLUMNS

One of the important applications of dynamic simulation is in relation to control and comparison of various control configurations for an existing or proposed system design. It enables the study of the dynamic response of the system to various disturbances which can be very valuable for the control system analysis and development.

Simulation of distillation columns, especially for control, can be divided into two parts:

(i) the preparation of a mathematical model of the distillation process

(ii) the use of the model to study control of the process

The mathematical modelling of tray distillation columns essentially involves the description of the unsteady state heat and mass transfer phenomena occurring on an individual stage and stepping this up from a single stage to a column with a number of similar stages to provide an approximation to the dynamic behaviour of the column. As regards stagewise distillation five different types of mathematical models can be used to describe the transient behaviour of a single tray : these models can be based upon:

(i) a perfectly mixed tray

(ii) plug flow across a tray : this is more relevant to bubble cap and valve trays than sieve trays

(iii) a perfectly mixed tray with time lag in the downcomer

(iv) longitudinal dispersion across a tray

(v) longitudinal dispersion with dead zones on a tray

All of these models except (i) and (iii) involve partial differential equations which are rather complex and require further simplifying assumptions, such as a linear equilibrium relationship, for solution. However, models (i) and (iii), in addition to being more flexible, also enjoy the advantage of being compatible for solution in the time domain by analogue and digital computers.

Both analogue and digital computer simulations of distillation columns have been attempted by different authors with varying degrees of success. Some of the earliest analogue simulation studies were those of Rose and his associates (76,77), who used an analogue computer to represent a five-tray column plus external control devices. Their work is indicative of the fact that analogue simulation of distillation columns can be very laborius and, when large columns are being investigated, the sheer number of analogue components required for a realistic representation of a column can be obtrusive and may, indeed, render the practice impossible.

This is the reason why analogue simulation is less attractive than its digital counterpart where the speed, flexibility and power of digital computers allow detailed dynamic simulations with relatively more ease. Some

of the earliest digital simulation attempts have been due to Rosenbrock (78,79,80), who introduced a computer procedure to solve large sets of simultaneous, non-linear differential equations so as to find the time needed for a column to reach its steady-state after it is started. Since the equations used were the original ones, without restricting assumptions, input step changes of any size could be introduced after the steady state had been reached and the response of the column could be observed.

As far as this thesis is concerned attention will be focussed on the review of the literature on the dynamic simulation of distillation columns using the perfectly mixed plate model, since they are more amenable to solution by digital computers.

II.3.1 SIMULATIONS BASED UPON UNSTEADY STATE MASS AND ENERGY BALANCES

The prefectly mixed plate model has been presented in various forms by several authors (76,77,78). The usual assumptions made in these derivations are:

(i) the liquid on each plate is perfectly mixed

(ii) the time constants for fluid and thermal transfers are negligible compared to that for mass transfer

(iii) vapour holdup is negligible compared with liquid holdup

(iv) the column is essentially adiabatic

(v) the steady-state efficiency does not change during transient periods

(vi) the liquid holdup on the plate is constant, i.e. the liquid and vapour holdups are not affected during transient periods.

The plate model is then derived by writing unsteady state material and energy balances across the plate.

In the case of binary distillation, the additional assumption of equimolal overflow is usually made to eliminate the need for the energy balance.

In what appears to be a refinement of this approach, more recently, various authors such as Franks (2) and Ramirez (5) have proposed the following equation for the calculation of the liquid overflow rate from each stage:

$$\tau \frac{dL_n}{dt} = L_{n-1} - L_n \quad \text{..... II.3.1}$$

where

L_n = liquid rate leaving the nth stage

L_{n-1} = liquid rate entering the nth stage

τ = hydraulic time constant

This equation is derived from a momentum balance on the liquid phase as illustrated by Ramirez (5).

Waggoner and Calvin (81) developed a simulation for a distillation column with the following characteristics:

(i) a stage-to-stage computation

(ii) a two component approximation to reduce the computation time

(iii) equilibrium described by specified stage relative volatility

(iv) overflow response developed from hydraulic effects

(v) minimal or no iteration within the time step

(vi) boil-up response that only shows a time lag in the reboiler

The programme developed by them included a numerical approximation for the time varying term in the material and energy balances.

Also, the equilibrium coefficient which is a non-linear function of the composition was recomputed whenever the composition changed. They have not produced any quantitative results to enable an assessment of such an approach.

II.3.2 SIMULATIONS INCLUDING FLUID DYNAMICS

The major criticism that may be raised against the previous approach to the dynamic simulation of distillation columns is the assumption of constant liquid holdup on the plates, since during throughput changes, the vapour and liquid rates and hence the plate holdups are expected to vary with time. Thus, although the assumption of constant liquid holdup may have little effect on the steady-state operation, dynamically, it appears unrealistic - particularly in the face of feed and reflux rates changes.

In order to remove this assumption, one has to resort to the consideration of the fluid dynamic phenomena occurring on a plate during operation. Luyben (3), and Lamb and his co-workers (82) have suggested that an unsteady state material balance should be made over each plate and that the liquid overflow rate from each plate should be calculated from the Francis (1) weir formula, i.e.

$$\frac{dM_n}{dt} = (L_{n-1} - L_n) + (V_n - V_{n-1}) \quad \text{..... II.3.2}$$

$$L_n = f \text{ (weir height, crest length and g)} \quad \text{. II.3.3}$$

where

M_n = holdup on plate n

L = liquid rate

V = vapour rate

It must be pointed out that the calculation of the liquid overflow by this method is only approximate, but it is simple and easy to use provided that the tray time constant is available or that it can be measured.

II.4 ESTIMATION

Multivariable control systems designed using state-space techniques often require that all of the system state variables be available to control the system. However, in many practical problems it may not be economical or convenient to measure all of the state variables. An alternative approach is to use an estimation technique to provide estimates of the state variables which are not measured. Kailath (83) gives a comprehensive review of the development of linear estimation theory during the past three decades while Rhodes (84) produces a useful tutorial introduction to estimation.

Of all the state estimation methods proposed in the literature, the Kalman filter (87,88,89) and the Luenberger observer (85,86) have received the most attention. Despite successful applications of the Kalman filter in the aerospace industry, there have been very few reported applications in the process industries (90,91). Similarly, few if any experimental applications of the Luenberger observer have been reported.

Both continuous-time and discrete-time forms of the Kalman filter are available (Jazwinski (16)). As regards this thesis, however, attention will be focussed upon the discrete-time version of the Kalman filter and its extended form : the so-called extended Kalman filter.

II.4.1 KALMAN FILTERING

The derivation of the Kalman filter has been reported by many authors (9,16). The discrete-time Kalman filter is composed of matrix recursion relations, the simplicity of which makes them particularly amenable to implementation on a digital computer. The requirements for a Kalman filtering exercise are:

(i) a lumped parameter model of the system in the time domain, i.e. a model comprising n linear differential equations

(ii) measurement statistics, i.e. the degree of uncertainty in the measurements

(iii) a good idea of the intensity of the random disturbances to which the system is exposed

(iv) the model accuracy statistics

The Kalman filter algorithm provides an optimal estimate of the state of a linear, time-variant dynamic system observed sequentially in the presence of additive Gaussian noise; such systems are referred to as linear stochastic dynamic systems. The estimate obtained at each sample time is optimal in the sense that it is the maximum likelihood estimate conditioned on all observations up to that time. Such a system can be described by the linear stochastic differential equation:

$$dx_t = A(t)x_t dt + D(t)u_t dt + G(t)d\beta_t$$

$$y_t = M(t)x_t + V_t \qquad \text{..... II.4.1}$$

where

t denotes time

x = vector of state variables (nxl)

y = vector of measured variables (mxl)

v = vector of random measurement disturbances, represented by a zero mean, white Gaussian noise process (mxl)

u = vector of deterministic system inputs (qxl)

A = continuous matrix time-function (nxn)

D = continuous system input driving matrix (nxq)

G = continuous matrix time-function (nxr)

and

$\{\beta_t, t \geq t_o\}$ is an r-vector of Brownian motion or Weiner process (16)

with

$$E\{d\beta_t \; d\beta_t^T\} = F(t).dt \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{II.4.2}$$

where

F(t) is a rxr continuous time-function matrix

Equation II.4.1 can now be integrated over the interval $\{t_k, t_{k+1}\}$ to convert the system into the discrete form.

$$x(t_{k+1}) = \Phi(t_{k+1}, t_k)x(t_k) + \int_{t_k}^{t_{k+1}} \Phi(t_{k+1},\tau)\, D(\tau)u_\tau .d\tau + \int_{t_k}^{t_{k+1}} \Phi(t_{k+1},\tau)G(\tau).d\beta_\tau \quad \ldots\ldots\ldots\ldots \text{II.4.3}$$

where the (nxn) matrix Φ is the state transition matrix, i.e.

$$\frac{d}{dt}\Phi(t,\tau) = A(t)\,\Phi(t,\tau) \quad \text{..... II.4.4}$$

where

$$\Phi(\tau,\tau) = I$$

$$\Phi(t,\tau)\,\Phi(\tau,\zeta) = \Phi(t,\zeta) \text{ for all } t,\tau,\zeta$$

also

$$\Phi^{-1}(t,\tau) = \Phi(\tau,t)$$

We can now write

$$W_{t_{k+1}} = \int_{t_k}^{t_{k+1}} \Phi(t_{k+1},\tau)G(\tau).d\beta_\tau \quad \text{..... II.4.5}$$

Thus

$$x(t_{k+1}) = \Phi(t_{k+1},t_k)x(t_k) + \int_{t_k}^{t_{k+1}} \Phi(t_{k+1},\tau)D(\tau)u_\tau.d\tau + W_{t_{k+1}}$$

..... II.4.6

where

$\{W_{t_{k+1}}\}$ is an n-vector of random system disturbances represented by a zero mean white Gaussian process.

Assuming that the deterministic system inputs are time-invariant between time t_k and t_{k+1} and for generality, let us also assume that there exists a discrete system noise coefficient matrix $\Gamma(t_k)$. We can then write

$$x(t_{k+1}) = \Phi(t_{k+1},t_k)x(t_k) + \Gamma_D(t_k)u(t_k) + \Gamma(t_k)W_{t_{k+1}}$$

..... II.4.7

$$Y(t_k) = M(t_k) + V_{t_k} \quad \text{..... II.4.8}$$

where

$\Phi_{t_{k+1}}$ = the state transition matrix (nxn)

$\Gamma_D = \int_{t_k} \Phi(t_{k+1}, \tau_k) D(\tau).d\tau$ the discrete input driving matrix (nxq)

$M(t_k) = M(t)$ the discrete measurement matrix (mxn)

Γ = system noise coefficient matrix (nxr)

W_{t_k} = r-vector of random system disturbances represented by a zero mean white Gaussian noise

For time invariant systems $\Phi = \exp(A\delta t)$

where $\delta t = t_{k+1} - t_k$

Also

$$E\{W_{t_k}\} = 0$$

$$E\{V_{t_k}\} = 0$$

For simplicity of notation we will henceforth represent the discrete time t_k by k. The respective covariances of V_k and W_k are given by:

$Q(k) = E\{W_k W_k^T\}$; the (nxn) system noise covariance matrix

$R(k) = E\{V_k V_k^T\}$; the (mxm) measurement noise covariance matrix

where

Q(k) and R(k) are positive semi-definite and positive definite respectively

Finally, assuming that the initial state estimate $x(0,0)$ together with its error covariance, $P(0,0)$ are known a priori, then the Kalman filter determines the estimate of the state and minimizes the quantity J as follows:

$$J = \tfrac{1}{2}\{\bar{x}(k)-x(k,k)\}^{T} P(k,k)^{-1} + \tfrac{1}{2}\sum_{i=1}^{k-1} \{y(i+1)-M(i+1)x(i+1,i)\}^{T} R(i+1)^{-1} \{y(i+1)-M(i+1)x(i+1,i)\} \quad \text{..... II.4.9}$$

where

$\bar{x}(k)$ is the true state of the system

$x(i,\ell)$ denotes the estimate of the state x at time i given the measurements up to time ℓ where $\ell<i$

$P(i,\ell)$ denotes the covariance of the error in this estimate

The filter variables are:

Variable	Definition	Dimension
$x(k,k)$	State estimate of t_k given $y(k)$	nxl
$p(k,k)$	Covariance matrix of error in $x(k,k)$	nxn
$\Phi(k+1,k)$	State transition matrix (from t_k to t_{k+1})	nxn
$\Gamma_D(k)$	System input driving matrix	nxq
$Q(k+1)$	System noise covariance matrix	rxr
$x(k+1,k)$	State estimate at t_{k+1} given $y(k)$	nxl
$P(k+1,k)$	Covariance of the error in $x(k+1,k)$	nxn

Variable	Definition	Dimension
M(k+1)	Measurement matrix	mxn
R(k+1)	Measurement noise covariance matrix	mxm
K(k+1)	Filter (Kalman) gain matrix at t_{k+1}	nxm
y_{k+1}	Measurement or observation at t_{k+1}	mx1
$\Gamma(k)$	System noise coefficient matrix	nxr

By examination of equation II.4.13 it can be seen that the estimate of the state vector x(k+1,k+1), is the sum of the predicted state and the weighted measurement error, K(k+1){y(k+1)-M(k+1)x(k+1,k)}. The original derivation of the algorithm (92) points out a number of valuable features of estimates thus calculated. These are that the estimate is uniformly asymptotically stable and that the convergence of the variances of the estimates, as each measurement is processed, is insensitive to round-off errors, provided that the system is observable and controllable.

The dual concept of observability and controllability were introduced by Kalman (92) in his original work as a part of his general filtering theory. Coggan and Noton (93) interpret these concepts as follows:

(i) a system is observable, if with perfect measurements and no random disturbances, all the state variables can be estimated after a finite number of measurements

(ii) a system is controllable if all the states are excited by the random disturbances Z(k)

II.4.2 THE KALMAN FILTER ALGORITHM

The Kalman filter algorithm can be written as a set of prediction and estimation equations as follows:

Prediction:

$$x(k+1,k) = \Phi(k+1,k)x(k,k)+\Gamma_D(k)u(k) \quad \ldots\ldots \text{II.4.10}$$

$$P(k+1,k) = \Phi(k+1,k)P(k,k)\Phi^T(k+1,k)+ \Gamma(k+1,k)Q(k+1)\Gamma^T(k+1,k) \quad \ldots\ldots \text{II.4.11}$$

Estimation:

$$K(k+1) = P(k+1,k)M^T(k+1).\{M(k+1)P(k+1,k)M^T(k+1)+R(k+1)\}^{-1} \quad \ldots \text{II.4.12}$$

$$x(k+1,k+1) = x(k+1,k)+K(k+1)\{y(k+1)-M(k+1)x(k+1,k)\} \quad \ldots\ldots\ldots\ldots \text{II.4.13}$$

$$P(k+1,k+1) = \{I-K(k+1)M(k+1)\}P(k+1,k) \quad \ldots\ldots\ldots \text{II.4.14}$$

or

$$P(k+1,k+1) = \{I-K(k+1)M(k+1)\}.P(k+1,k)\{I-K(k+1)M(k+1)\}^T + K(k+1)R(k+1)K^T(k+1) \quad \ldots\ldots\ldots \text{II.4.15}$$

The more important concept to the field of filtering theory is that of observability. If one of the state variables of the system cannot affect the measurement vector then the consequential unobservability leads to the estimates produced by the filter being sub-optimal.

The time taken for the filter to converge has been shown by Storey (94) to depend on the accuracy of the

initial estimate, $x(0,0)$, and the initial error covariance, $P(0,0)$, a priori knowledge of which is required to initiate the filter. The larger the initial error in the estimates, the longer the filter takes to converge. This is because until the system has become observable, the filter relies on the initial estimate. In the case of a large initial error covariance matrix, the filter will display a slower response since it will rely initially upon current noisy measurements.

In the statement of the filter algorithm, alternative equations have been given for determining the error covariance of the state estimations (equations II.4.14 and II.4.15). It has been shown by Aoki (108) that equation II.4.15 is preferable since the right hand side is the sum of two symmetric positive definite matrices while equation II.4.14 is at best the difference of two positive definite matrices. Therefore, equation II.4.15 is better conditioned for numerical computation and will retain the positive definiteness and symmetry of $P(k,k)$.

Following the original work of Kalman, the main contributions to the field of linear filtering theory have been aimed at generalizing Kalman's earlier work. The most significant of these developments (95,96) have been in extending the theory to allow for correlation between the system and measurement noises. The problem of coloured (time-correlated) is partially solved by Kalman (97). Jazwinski (16) provides a comprehensive review of these generalizations.

II.4.3 EXTENDED KALMAN FILTER

The Kalman filter formulation is in terms of a linear state-space model and is thus only applicable to systems which can be described by a set of first order, linear differential equations and in which the outputs are linearly related to the state variables. For such systems the theory developed by Kalman provides an optimal filter. To most engineering problems, however, such a linear model is not immediately applicable except as a very rough approximation. The dynamic system for most engineering problems is frequently found to be described by a series of nth order differential equations. The fact that nth order derivatives appear does not offer any theoretical difficulties because any nth order differential equation may be written as a system of n first order differential equations. Nonetheless, the output of the system commonly appears in terms of quantities that have a non-linear algebraic relation with the state variables and thus the application of the Kalman filter to such systems may seem illogical due to its completely linear basis. However, its computational ease and conceptual simplicity has led to a modification of the Kalman filter which is commonly referred to as the extended Kalman filter. The application of the extended Kalman filter to non-linear systems is essentially characterized by the following points:

(i) it requires linearization around each last estimate prior to the next estimation by Taylor series expansion neglecting the second and higher order terms

(ii) if the state variables are not being measured directly, instead of the "state" and "measurement", we then consider the state deviation and the measurement deviation from a reference trajectory which is physically meaningful. The choice of the latest estimated state or the steady state as the reference trajectory is not uncommon

(iii) the estimates may no longer be optimal

Consider the non-linear stochastic system described by

$$dx_t = F(x_t,u_t)dt + G(t)d\beta_t \quad \text{..... II.4.16}$$

$$y_t = H(x_t) + V_t \quad \text{..... II.4.17}$$

or the discrete form

$$x_{k+1} = f(x_k,u_k) + \Gamma(k)w_{k+1} \quad \text{..... II.4.18}$$

and observations

$$y_k = h(x_k) + v_k \quad \text{..... II.4.19}$$

where β,u,v and w are as defined for the linear system.

If the system equations are linearized about the current estimate of state x_k, by means of a truncated Taylor series expression (16), the linear Kalman filter algorithm is applicable except:

(i) the state prediction stage is carried out as

$$x(k+1,k) = x(k,k) + \int_{o}^{\delta t} F(x_t,u_t).dt \quad \ldots\ldots\ldots \text{II.4.20}$$

where

$x(k,k)$ is the estimate of state at t_k

$$\delta t = t_{k+1} - t_k$$

(ii) the state transition matrix may be approximated by

$$\Phi(k+1,k) = I + \frac{\partial f(x_k,u_k)}{\partial x_k}.\delta t \quad \ldots\ldots\ldots\ldots \text{II.4.21}$$

where the Jacobian $\frac{\partial f(x_k,u_k)}{\partial x_k}$ is evaluated about the latest estimated state or a predetermined reference trajectory.

(iii) the measurement matrix is evaluated as

$$M(k+1) = \frac{\partial h(x_k)}{\partial x_k} \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{II.4.22}$$

where the derivatives are evaluated about a reference trajectory or the latest estimated state.

Notation

x_t	continuous variable
$x(t_k)$	discrete variable
$x(k)$ and x_k	abriviations for $x(t_k)$
H,f	continuous time functions
h,f	discrete time functions

II.4.4 ESTIMATION APPLIED TO CHEMICAL PROCESSES

Applications of estimation to chemical processes have been predominantly concerned with Kalman filtering. Webb (27) gives a comprehensive review of the work done in this area - particularly in open loop situations. Of interest to this thesis is the use of estimation in closed-loop or control situations and thus we will concentrate on review of the work on this aspect of estimation.

One of the most notable of the earlier chemical engineering applications of the Kalman filter was by Noton and Choquette (98,99) in the identification of a reactor train. The initial work was done using an off-line computer applied for open loop control experiments. Following the success of these experiments further work was done during closed loop experiments using a remote time-sharing computer. Although this work cannot be described as an on-line application, the overall exercise was successful inasmuch as a significant improvement over manual control was reported.

The theoretical problems encountered when dealing with systems containing a large number of state variables, unknown parameters, transport lags and strong non-linearities was tackled with considerable success by Coggan and Noton (93). In this paper the extended Kalman filter is applied to simulated systems exhibiting large random disturbances and having unknown initial values. The possibility of trading model simplification for

unnecessary numerical accuracy is also discussed.

An approach to model reduction is suggested by Coggan and Wilson (100), who minimise the number of state variables required to describe a system. The extended Kalman filter is modified to evaluate measurement error statistics and detect the presence of bias. The same authors also report the on-line implementation of this filter. The mini computer used had 4k words of memory and was applied to a tenth order system.

Most of the work reviewed by Webb (27) is concerned with open-loop state and parameter estimation. Lynch and Ramirez (101), however, were one of the first groups of workers who investigated estimation in a closed-loop control situation. They developed and implemented a time-optimal control algorithm for a continuous stirred tank reactor. Estimation was carried out by an extended Kalman filter. The reaction studied is the decomposition of hydrogen peroxide with a homogeneous catalyst of potassium iodide. The experimental work done was in an on-line environment using a General Data Corporation Nova 1210 Minicomputer with 8k words of memory. Lynch and Ramirez conclude that extended Kalman filter works very well in estimating the unmeasured system states of the non-linear model. The authors do not implement the complete filter algorithm in an on-line situation. The filter gain matrix, K, is assumed to be constant for a system at or near steady-state and is computed off line from a steady-state value of the estimation error covariance matrix, $P(k,k)$.

The first experimental studies of the on-line implementation of non-stationary forms of the Kalman filter are reported in the work by Payne (28) and Coleby (29). Both of these workers studied the on-line, real-time implementation of an essentially uncontrolled double effect evaporator, whose instrumentation was interfaced to a Honeywell 316 computer with 16k words of memory.

The earlier work of Payne was involved with the application of the extended form of the Kalman filter. His work highlighted the many difficulties that are encountered during on-line implementation of the Kalman filter, many of which have been overlooked by workers involved in simulated studies. Two of the most important points are the cycle time required by the filter algorithm for large systems and the assumptions required in order to make the system operate within the limits imposed by the equipment used.

Following the work of Payne, the problem of a poor system model was tackled by Coleby. Coleby states that where there is doubt about the accuracy of the prediction equations, some method to control the filter divergence should be incorporated into the filter algorithm.

A complete experimental study of modern control theory was carried out during the years of 1972 to 1974 by Soberg, Fisher and co-workers in the Department of Chemical Engineering at the University of Alberta in Canada. The research carried out was specifically

concerned with the implementation of computer control of a pilot plant size, double effect evaporator and the subsequent evaluation of multivariable design techniques. In a collective report (102) the authors indicate that the incorporation of the Kalman filter into a multivariable computer control system provides significantly better control. It is significant to note that these workers used the noise covariance matrices R and Q as design parameters. This indicates that the on-line application of the Kalman filter involves a certain amount of "tuning".

More recently, Litchfield and co-workers (116) applied five different Kalman filters to the problem of estimating the state of a real chemical reactor operating under open-loop and feedback control. The filters considered included the fixed gain, the extended and the exponentially data weighted. It is significant that they conclude that the extended Kalman filter was the most successful when used in open-loop and feedback time-optimal control schemes.

II.4.5 ESTIMATION APPLIED TO DISTILLATION COLUMNS : THE COMPUTER PATH

The earliest attempt to apply estimation to distillation columns were those of Brosilow and Weber (34), who proposed a linear static least square estimator to relate perturbations in the measured quantities to perturbations in product quality. The estimator is derived from a linear model of the process which is valid in some region about a steady-state operating point. The implication of this is that the static estimator is only applicable to cases with mild non-linearities or small deviations from the steady state.

Luyben and Shah (106), in pursuit of this proposal, used a non-linear estimator to control a binary distillation column and found that estimator-based schemes achieved superior composition control to that achieved with conventional control schemes.

More recently, in a series of three papers, Brosilow and his co-workers (103,104,105) introduced the notion of Inferential Control which essentially means using selected temperature and flow measurements to estimate, or infer, the effect of measurable disturbances on product quality and adjust the control effort to counteract the effect of the measured disturbances. It must be pointed out that although these static estimators can be made insensitive to modelling and measurement noises, they propose no means of improving an inaccurate model and are solely intended

for the estimation of product compositions from secondary measurements. These authors also consider the use of optimal dynamic estimators. However, the fact that they attempt to analyse the estimators in the Laplace domain tends to obscure the issue to some extent since it is generally believed that the dynamic estimators are best analysed and understood in the time domain.

A thorough experimental investigation of the available control schemes for distillation columns has been carried out by Dahlqvist (107). He measured the compositions on various plates and used the Kalman filter for state reconstruction that is needed for multivariable feedback controller design. It is significant that he reaches the following conclusions:

(i) multivariable controllers designed from purely theoretical models give better results than the SISO controllers that were tuned on-line to the process

(ii) coupling of reflux flowrates to boil-up proved to be effective when there was an unmodelled time delay in the system

(iii) a third composition measurement located near the feed tray improves the performance of the control system

(iv) the control variables are faster adjusted to new steady state levels if feedforward compensation is applied

It appears, however, that by using the Kalman filter off-line and for state reconstruction only, he

does not exploit the full potential of the Kalman filter - especially for on-line applications.

NOTATION

$\underline{A}$ = relating matrix

$\underline{B}$ = the matrix of left eigen vectors of $\underline{A}$

B = bottoms rate

B_1, B_2, B_3 = temperature measurements near the feed plate, an intermediate temperature and bottoms temperature respectively

$\underline{C}$ = the matrix of right eigen vectors of $\underline{A}$

C_p = molar specific heat capacity

D = distillate

$\underline{D}$ = driving matrix

F = feed rate

Z = feed composition

G_C = controller transfer function

G_V = valve transfer function

G_M = measurement transfer function

J = scalar performance criterion

$\underline{K}$ = proportional gain matrix

L_n = liquid leaving the nth tray

$\underline{P}$ = plant matrix or the Ricatti matrix

$\underline{Q}$ = positive semi definite weighting matrix

$\underline{R}$ = weighting matrix

R = reflux rate

R_I = internal reflux

S = separation factor

T_o = overhead temperature

T_r = reflux temperature

$\underline{u}_i$ = eigen vectors of $\underline{A}^T$

$\underline{u}(t)$ = control effort

$\underline{V}_i$ = eigen vectors of $\underline{A}$

V_n = vapour rate leaving the nth tray

x = liquid compositon

y = vapour composition

$\underline{X}$ = vector of state variables

Subscripts

m = measured value

Greek Symbols

λ_i = eigen values of $\underline{A}$

τ = hydraulic time constant

Filtering Notation

A = continuous matrix time function

D = continuous system input driving matrix

G = continuous matrix time function

K = filter gain matrix

$M(t)$ = continuous measurement matrix

$M(t_k)$ = discrete measurement matrix

P = error covariance matrix

Q = system noise covariance matrix

R = measurement noise covariance matrix

t = continuous time

t_k = discrete time

u = vector of deterministic system inputs

v = vector of white Gaussian noise

w = vector of random system disturbances represented by a zero mean white Gaussian process

x = vector of state variables

y = vector of measured variables

Greek Symbols

β_t = vector of Brownian motion or Weiner process

ϕ = state transition matrix

Γ = system noise coefficient matrix

Γ_D = discrete system input driving matrix

C H A P T E R T H R E E

THE CONSTRUCTION AND INSTRUMENTATION OF THE DISTILLATION COLUMN AND ITS INTERFACING TO THE HONEYWELL-316 COMPUTER

III.1 INTRODUCTION

The process equipment is shown in Figure III.1. It will be described through the following stages:

(i) the construction of the column

(ii) its instrumentation

(iii) its interfacing to the departmental Honeywell 316 computer via the Honeywell Analogue/Digital Input System (HADIOS)

The distillation column and its accessories were donated to the Department by the I.B.M., U.K. Ltd., together with some parts for its instrumentation and data conditioning.

All of the hardware involved will be described in this Chapter. The software associated with HADIOS will be discussed in Chapter V.

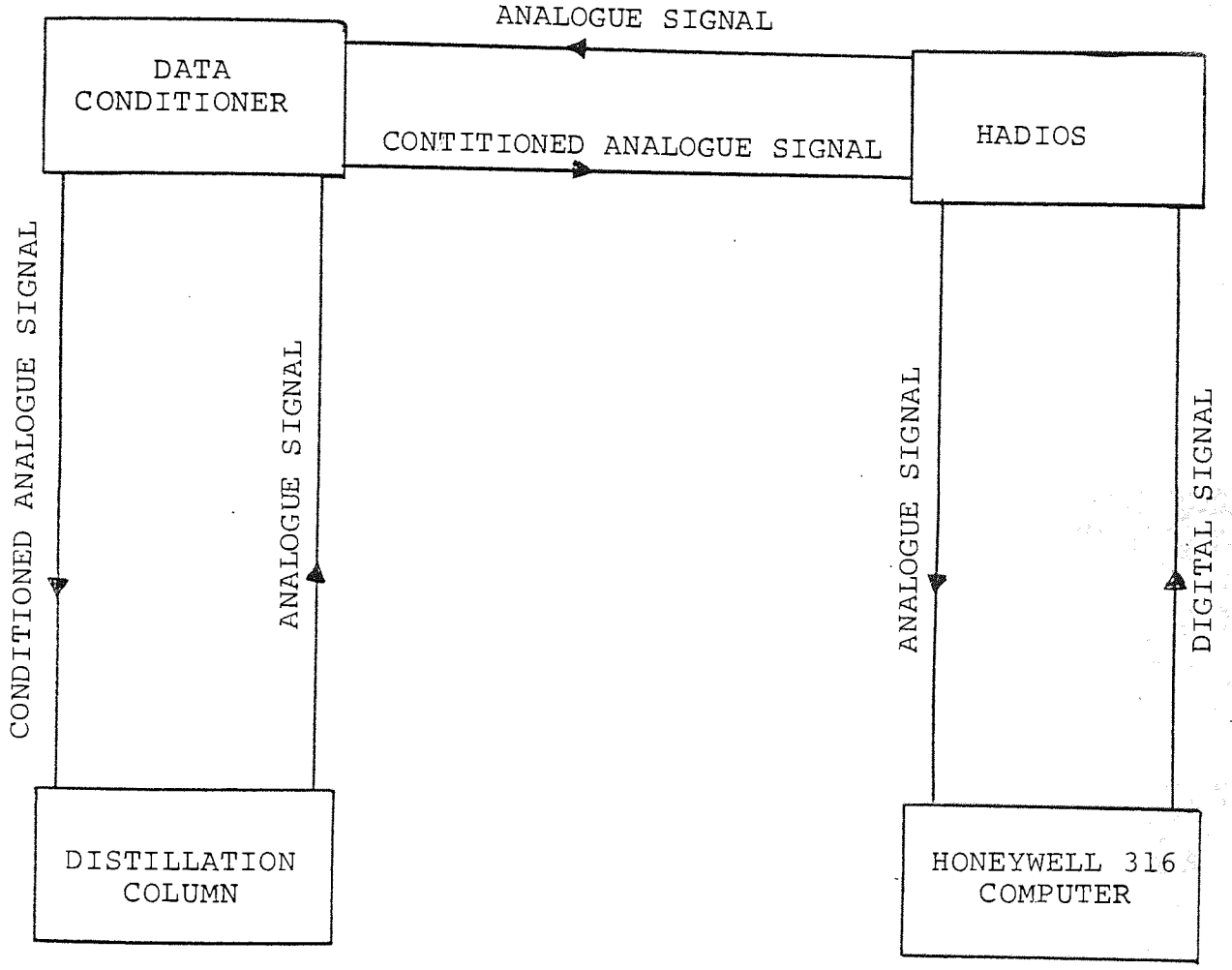


FIGURE III.1 - The Entire Experimental arrangement in Block Diagram

III.1.1 THE CONSTRUCTION OF THE DISTILLATION COLUMN

At present, the column and its accessories comprise:

(i) an enriching and a stripping section with six and four 3-inch diameter sieve trays respectively and one temperature measurement well per tray

(ii) a 3-inch diameter standard glass total condenser plus the reflux drum

(iii) a 2.4 kw, double-circuit Isomantle electric heater

(iv) a 1 metre long, 3-inch O.D. glass pipe section situated above the enriching section to enable gravity flow in the reflux and distillate lines

(v) two cylindrical feed tanks to enable composition changes to be introduced

(vi) a spherical top product tank

(vii) a spherical bottom product tank

(viii) three centrifugal stainless steel pumps

The schematic diagram of the column is given in Figure III.2 while that of a typical tray is depicted in Figure III.3. The column and tray's leading characteristics and dimensions are given in Tables III.1 and III.2 respectively.

The column was intended to be an all-purpose distillation column capable of handling corrosive liquids. Therefore, the materials used for its construction and piping were strictly limited to stainless steel, glass and P.T.F.E. All of the pipe lines are

made of ½ inch O.D. heavy gauge stainless steel with the exception of the overhead vapour line connecting the column to the condenser which is made of glass and is 3 inches in diameter.

The feed tanks have been situated at a relatively higher elevation from the feed pump so that the drop in the liquid level in the tanks does not affect the total head on the suction end of the pump appreciably and thus the flow through the feed line remains effectively constant during a run.

The condenser cooling water is supplied by a standard constant head tank. The cooling water is received from the departmental cooling tower.

A small heat exchanger has been installed in the bottom product line. Its purpose is to ensure that boiling liquid does not reach the pump and thus the likely pump cavitation problems are avoided. The cooling-water supply for this heat exchanger is also supplied by the departmental cooling tower.

The entire column and the vapour line from the column to the condenser have been lagged with ½" standard fibre glass lagging. Plates 1,2 and 3 show the entire column and its accessories from three different angles.

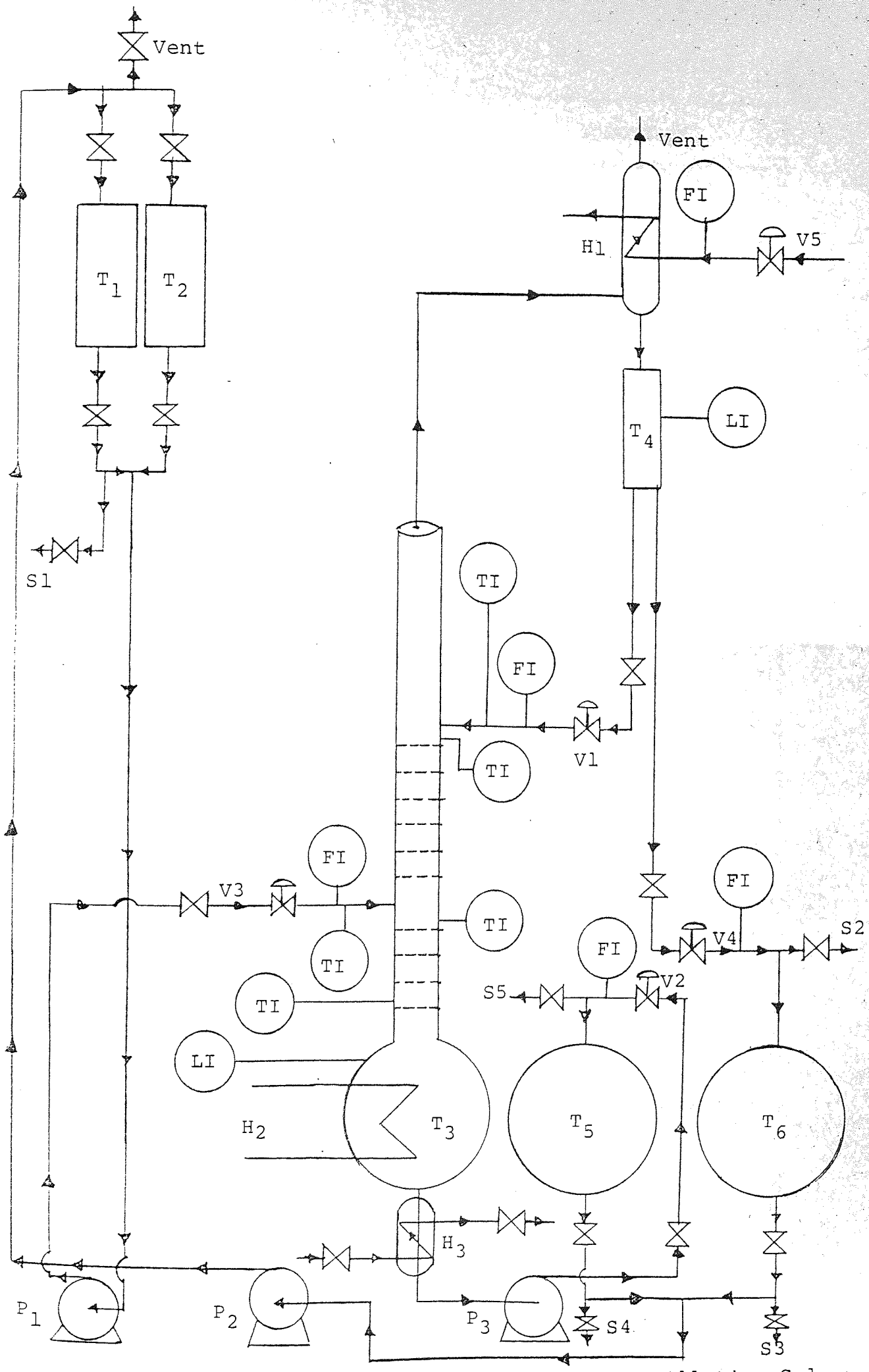


Figure III.2 - The Schematic Diagram of the Distillation Column

Process Notation	Function and Material	Dimensions
T_1 and T_2	Feed Tanks: glass	Volumes = 30 lit. approx.
T_3	Reboiler: glass	Diameter= .32 m. approx.
T_4	Reflux Drum: glass	Diameter= .762 m.
T_5	Bottoms Tank: glass	Volume = 50 lit. approx.
T_6	Distillate Tank: glass	Volume = 50 lit. approx.
V_i; i=1,5	Motorized Valves: stainless steel	
S_i; i=1,5	Sample Valves: stainless steel	
P_i; i=1,3	Centrifugal Pumps: stainless steel	
H_1	Total condenser: glass	Diameter= .762 m.
H_2	The Electric Heater	
H_3	Heat Exchanger	
TI	Temperature Indicator	
FI	Flow Indicator	
LI	Level Indicator	

Other Miscellaneous Dimensions:

Length of the enriching section = 0.65 m. approx.

Length of the stripping section = 0.55 m. approx.

Length of the gravity flow pipe = 1.0 m. approx.

Table III.1 - The Process Notation and Main Particulars of the Column

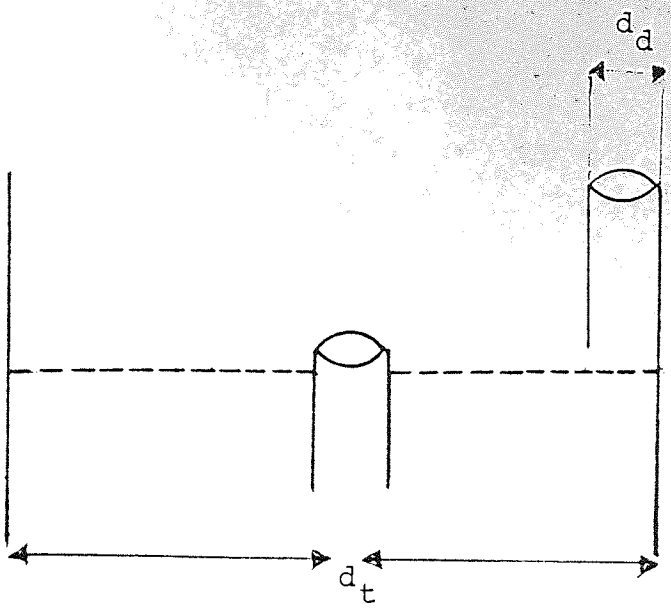


Figure III.3 - The Schematic Diagram of a Sive Tray in the Column

Diameter of the Tray	0.762 m
Diameter of the Downcomer	0.105 m
Tray Thickness	0.002 m
Diameter of the Perforations	0.0011 m
Number of Perforations	145 holes per tray
The Weir Height	0.003 m

Table III.2 - The Characteristic Dimensions of a Tray and Other Geometrical Information

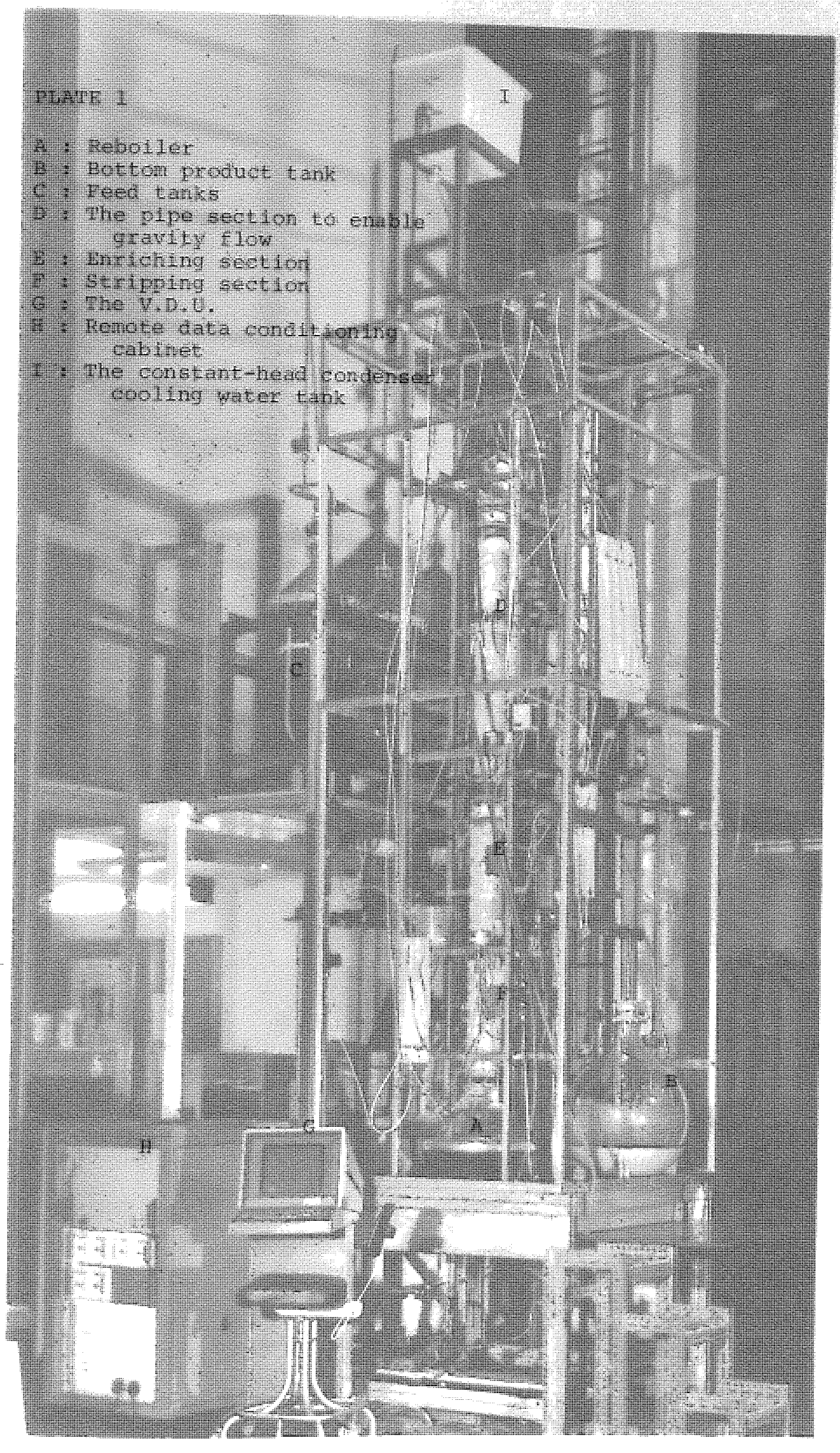


PLATE 1
A : Reboiler
B : Bottom product tank
C : Feed tanks
D : The pipe section to enable gravity flow
E : Enriching section
F : Stripping section
G : The V.D.U.
H : Remote data conditioning cabinet
I : The constant-head condenser cooling water tank
I
D
C
E
B
A
F
G
H

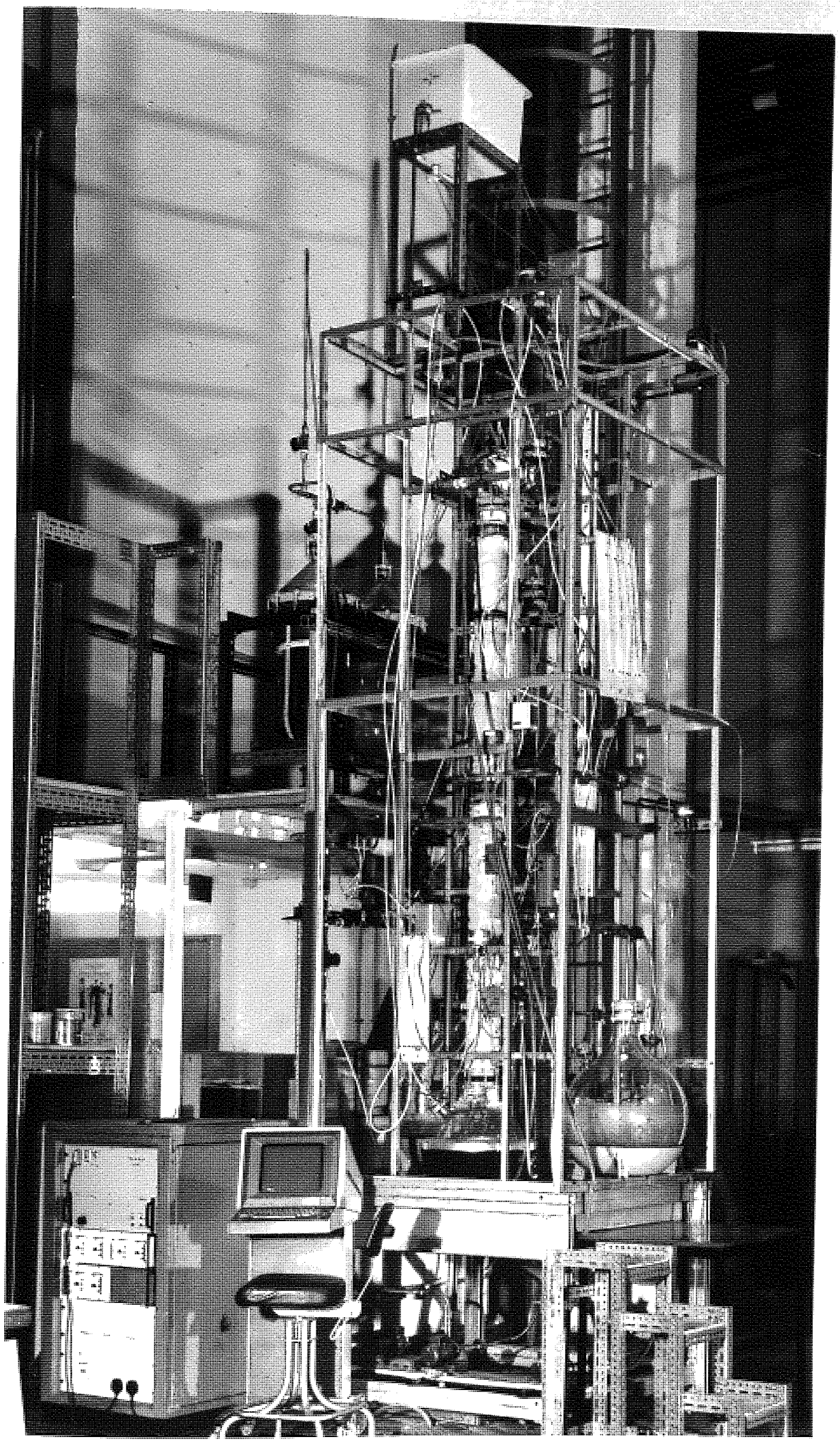
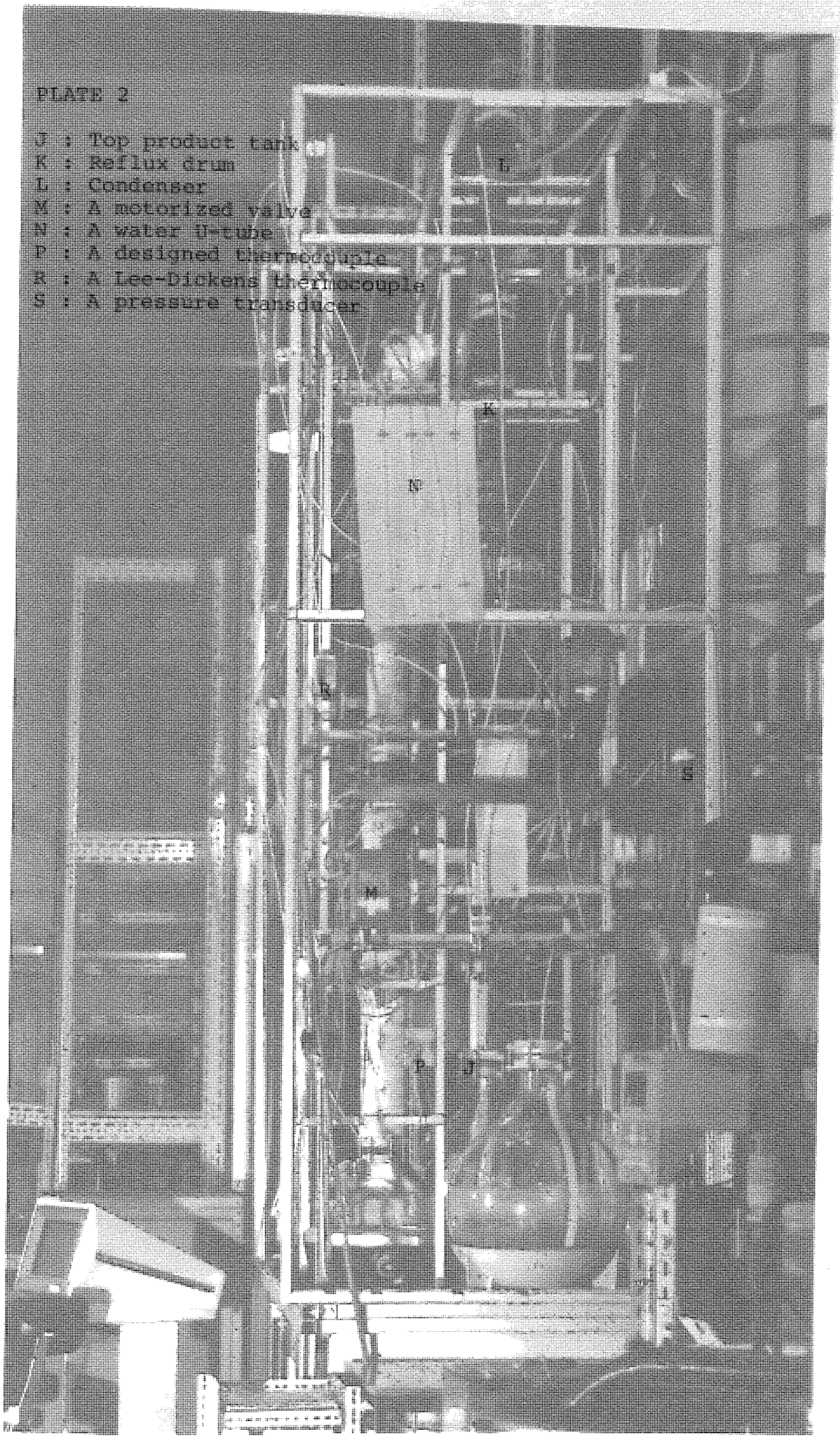


PLATE 2


J : Top product tank
K : Reflux drum
L : Condenser
M : A motorized valve
N : A water U-tube
P : A designed thermocouple
R : A Lee-Dickens thermocouple
S : A pressure transducer
J
K
L
N
M
P
R
S

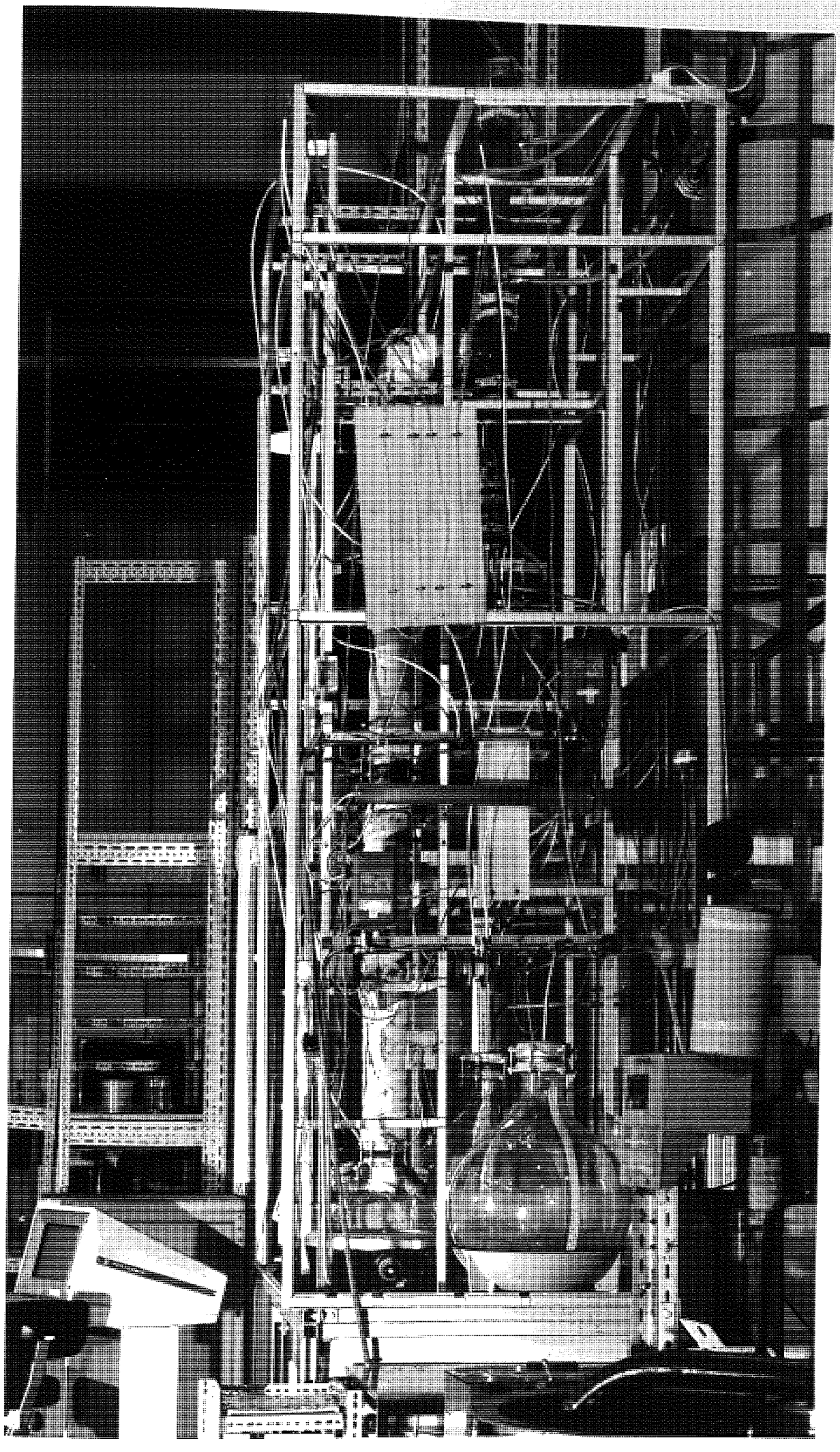
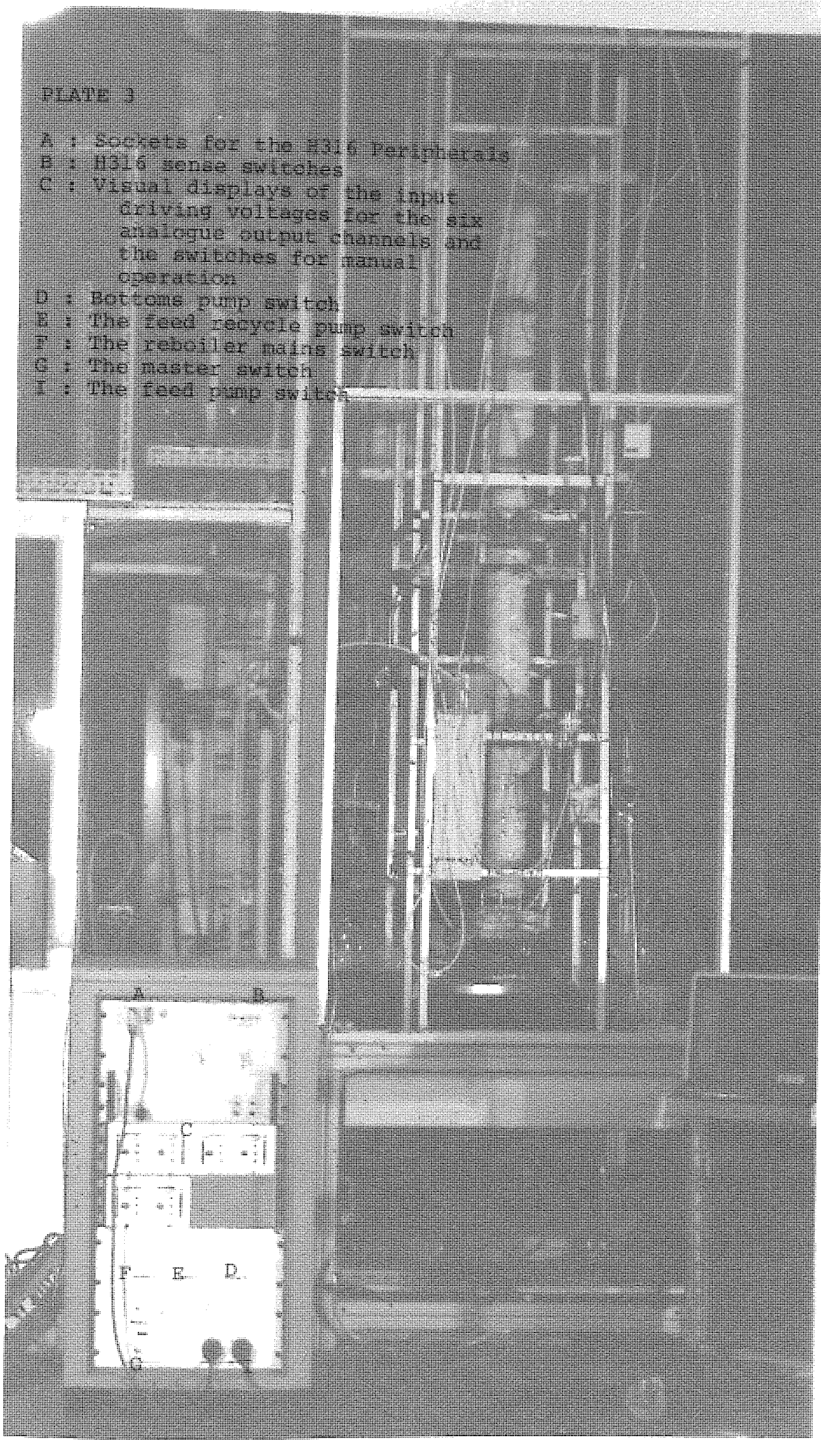
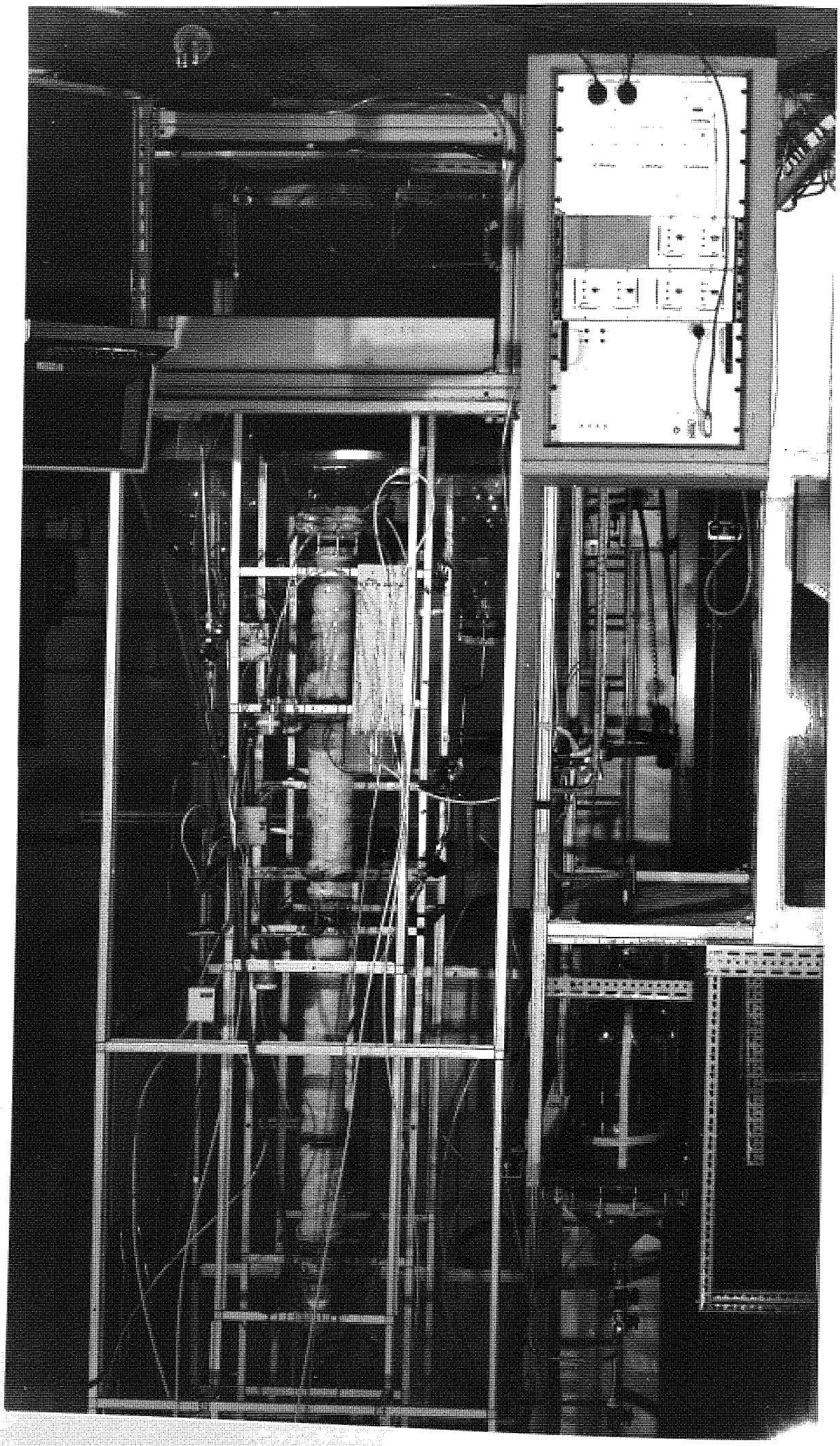


PLATE 3

A : Sockets for the 8316 peripherals
B : 8316 sense switches
C : Visual displays of the input driving voltages for the six analogue output channels and the switches for manual operation
D : Bottome pump switch
E : The feed recycle pump switch
F : The reboiler mains switch
G : The master switch
I : The feed pump switch





III.1.2 THE MOTORIZED VALVES

Liquid flow control by electric signal is done by an instrument known as Lek-Set which converts an electric signal into the mechanical adjustment of a flow control valve so that a desired liquid flow rate results from a specific input.

A software package known as the HADIOS Executive is available which enables analogue signals to be transmitted from the computer to the valves. Detailed discussion of HADIOS and its associated software will be given in due course in this Chapter and also in Chapter V.

The valves as presently installed on the column can, therefore, be driven automatically by a signal from the computer and, also, manually by pressing the appropriate switches on the panel of the remote signal conditioning unit positioned next to the distillation column (see the description of the interfacing of the column to H316 computer). Visual displays of approximate valve input signals have also been installed.

The response and shut-off characteristics of the valves were investigated by Daie (134) by side-bench experiments during which the valves were interfaced to the H316 computer individually and their characteristics were studied.

The shut-off characteristics of the valves can be modified to some extent by varying the length of

the valve needles, but complete shut-off is difficult to achieve. Therefore, each motorized valves is preceded by a manual valve to enable shut-off if need be.

The range of the input signals to the valve is 0 to 10 v. from fully closed to fully open stem positions. Their calibrations can be done insitu by outputting a signal from the computer and measuring the volumetric flowrate by stopwatch-and-bucket method. The output signal can then be correlated to the flow rate by the least squares method. The general form of the correlations is:

output voltage = g(volumetric flow rate) .. III.1

The order of the polynomial fit for each valve was increased until the variance about the regression plane was almost invariant with the increasing order of the polynomial. These calibrations were found to be reproducible provided no electrical or mechanical adjustments were made to the valves.

Table III.3 provides the coefficients of the equations describing the motorized valves while their characteristic curves are given in Appendix A.1.

Valve	a_i	b_i	c_i	d_i	e_i	α_i
Reflux	-0.08062	2.837	54.170	137.8	-	.998312
Bottoms	-0.843	14.9	-3.45	-	-	.989165
Feed	-0.04539	8.378	-2.732	-4.816	5.910	.996142
Distillate	0.405	49.2	-17.6	-	-	.988967

Table III.3 - The flow rates are in litres/min. and the voltages are in volts. α is the correlation coefficient and a_i ... e_i are the coefficients of the polynomials

Valve Operation Problems

The following types of stiction can occur during the operation of the motorized valves:

(i) electrical stiction; where the valves may literally not respond to changes in the input voltage of less than 1 volt

(ii) mechanical stiction; where the mechanical parts of the valves may stick because of dirt and lack of lubrication

The first of these problems can be overcome by programming a "kick" to be sent to the valves every time their settings are changed or refreshed. This effectively means that the valves are driven towards their maximum opening to shift them slightly and, then, reset to their desired opening immediately afterwards. In programming language, this can be accomplished by two consecutive CALLS to subroutine 5 in the latest version of HADIOS Executive.

The mechanical problems can only be reduced by constant lubrication and maintenance.

The hysteresis effects were found to be minimal over an operation time of two hours.

III.1.3 THE REBOILER

The reboiler is essentially a 2.4 kW, double circuit isomantle electric heater which can be driven by a maximum of 10 volts input voltage from the computer or manually.

The reboiler characteristics were studied insitu and it was found that for a certain input driving voltage, and a known mass of liquid, the temperature of the liquid rose linearly with time. This meant that the amount of heat transferred to the liquid, as calculated from equation III.2, could be conveniently correlated to the input signal.

$$Q = MC_p \frac{dT}{dt} \quad \text{..... III.2}$$

where

M = mass of the liquid in the reboiler

C_p = specific heat capacity of the liquid

Q = the rate of heat transfer

and $\frac{dT}{dt}$ is determined from the plot of temperature vs time

The experimental arrangement was as follows:

(i) a variable speed electric stirrer introduced into the reboiler through the available spouts on the reboiler

(ii) a precalibrated electric thermocouple

(iii) a stopwatch

The mass of water as the liquid used for calibration was chosen to be 12 kg. because it happened to have the optimum volume needed to cover the entire surface area between the electric coil and the spherical glass container.

This experiment was repeated for different input voltages and Q was calculated from equation III.2 for each experiment. It was, therefore, possible to correlate the input voltage to the amount of heat transferred as

The amount of heat transferred = g(input voltage)

..... III.3

or

$$Q = .3312 - 0.1772V + 0.07919V^2 - 0.005239V^3$$

where

Q = the heat transferred kj./sec.

V = input voltage volts

or alternatively

Input voltage = f(the amount of heat to be transferred)

..... III.4

$$V = 3.62 - 3.86Q + 6.59Q^2$$

As stated, during the calibrations the mass of the liquid was fixed at a level such that maximum heat transfer area was obtained. In actuality, the mass of liquid in the reboiler and thus the associated heat transfer area change during operation. Therefore, the heat transferred as calculated from equations III.3 and III.4 must be corrected for the variations in the heat transfer area. This correction factor

was obtained by fixing the input voltage to the reboiler and varying the mass of the liquid inside the reboiler and was found to be practically the same for any input voltage. Denoting this correction factor by R, it was correlated to the mass of the liquid contained by the following equations

$$R = g(\text{mass of liquid in the reboiler})$$

or $$R = -0.9183+0.4854M-0.04422M^2+0.001914M^3-0.00004078M^4 \quad \text{..... III.5}$$

where

$$R = \frac{Q_{12}}{Q_A}$$

Q_{12} = heat transferred when the mass of liquid in the reboiler is equal to 12 kg. as calculated from equation III.3

Q_A = the actual amount of heat transferred

The curve-fittings were done by the least squares method and the orders of the polynomials were increased until the variances about the regression plane were almost invariant with the increasing order of the polynomials.

The characteristics of the reboiler are given in Appendix A.2.

III.2 PROCESS INSTRUMENTATION

Low-cost instrumentation was one of the side objectives of this research since expensive instrumentation often acts as a deterrent against computer control. Therefore, low cost measurement methods had to be devised in an attempt to achieve this objective and thus reduce the cost to an acceptable level. The approach to these developments was essentially teleological in that these developments were made to serve certain purposes. However, there is no reason why they cannot be duplicated and employed effectively elsewhere.

The present instrumentation of the distillation column will be discussed in following parts:

(i) temperature measurement

(ii) level measurement

(iii) flow measurement

III.2.1 TEMPERATURE MEASUREMENTS

The Lee-Dickens Thermocouples:

These thermocouples were originally intended for plate temperature measurements on the column. Their calibrations, however, proved to be unduly cumbersome due to the fact that they were made up from very cheap and, thus, electrically primitive components such as low cost amplifiers and inherently drift-prone thermistors which constitute the automatic

zero compensation unit of the thermocouples.

At the outset, the scatter between consecutive readings amounted to ±12 percent. The calibrations were further invalidated by the following observations:

(i) the thermocouples gave different readings of the same nominal temperature

(ii) they actually changed in different directions. In other words, one thermocouple showed a fall in the temperature of a water-bath while the others indicated a rise

(iii) a ripple was observed in the output signal from the transducer when monitored on an oscilloscope

(iv) there was a drift in the calibrations, i.e. consecutive calibrations showed different offsets

The non-uniformity in the readings of the thermocouples was found to be due to the pick-up of noise from various sources. The following sources of noise were identified.

(i) the motorized valves are mains-operated and the interface between the mains and the driving signal from the Honeywell 316 was giving rise to a significant amount of noise which was readily being picked up by the thermocouples

(ii) there was high frequency digital noise from the Honeywell 316 computer which affected the transducers

(iii) there was noise pick-up from the internal power supply of the thermocouples.

These problems were further compounded by the fact that the impedances between the input to and output from the HADIOS were not properly matched and this, in turn, gave rise to additional inconsistencies in the calibration of the thermocouples.

The following remedies were conceived and implemented.

(i) the noise originating from the motorized valves was minimized by the installation of an external power supply solely for the thermocouples. This proved to be effective as it reduced the valve interference and the resulting noise considerably

(ii) the digital noise problem was overcome by the addition of a capacitor between the output from the H316 and input to the HADIOS

(iii) the impedances between the input to and the output from the HADIOS were matched by adding an amplifier between the output from the thermocouples and input to the HADIOS

(iv) the effect of transients caused by the internal power supply were alleviated by the following methods:

(a) the addition of a capacitor between the output from the thermocouples and the input to the HADIOS

(b) shortening the thermocouples as far as possible

(c) screening the thermocouples

Two lines of attack were available to overcome the problem of the ripple observed in the output signal from the thermocouples. These were:

(i) by more hardware modification involving the addition of a capacitor (integrator) to the feedback loop of the transducers

(ii) by a software modification to the HADIOS Executive such that the ripple would be averaged out over a period of time

The notion of further hardware modification was abandoned because the integration of the ripple by a capacitor meant that any faults in the thermocouples such as the drifts of the automatic zero compensation unit would also be integrated.

It was therefore decided to add a piece of software to the latest version of the HADIOS Executive MOD.2, to enable the ripple to be smoothed out by taking as many equally-spaced samples as possible during the entire scan interval - the details of which will be discussed in Chapter V.

Finally the problem of drift in the automatic zero compensation thermistor can be overcome by bypassing the thermistor and using the melting point of ice as the reference temperature.

The result of these modifications was to eliminate non-uniformities and enable the calibration to be

reproducible with an accuracy $\pm 1^{o}C$. This, however, was thought to be too inaccurate for tray temperature measurements and thus it was decided to use these thermocouples for the feed and reflux stream temperature measurements where the accuracy is not so crucial for open-loop experiments or control.

For tray temperature measurements, nonetheless, it is possible to get good accuracy and almost noise-free readings economically by the design proposed in Figure III.4, which has the following features:

(i) nickel-chromium aluminium thermocouples

(ii) high performance operational amplifiers known by the type number 725CN supplied by many manufacturers

(iii) long-life batteries used as internal power supply

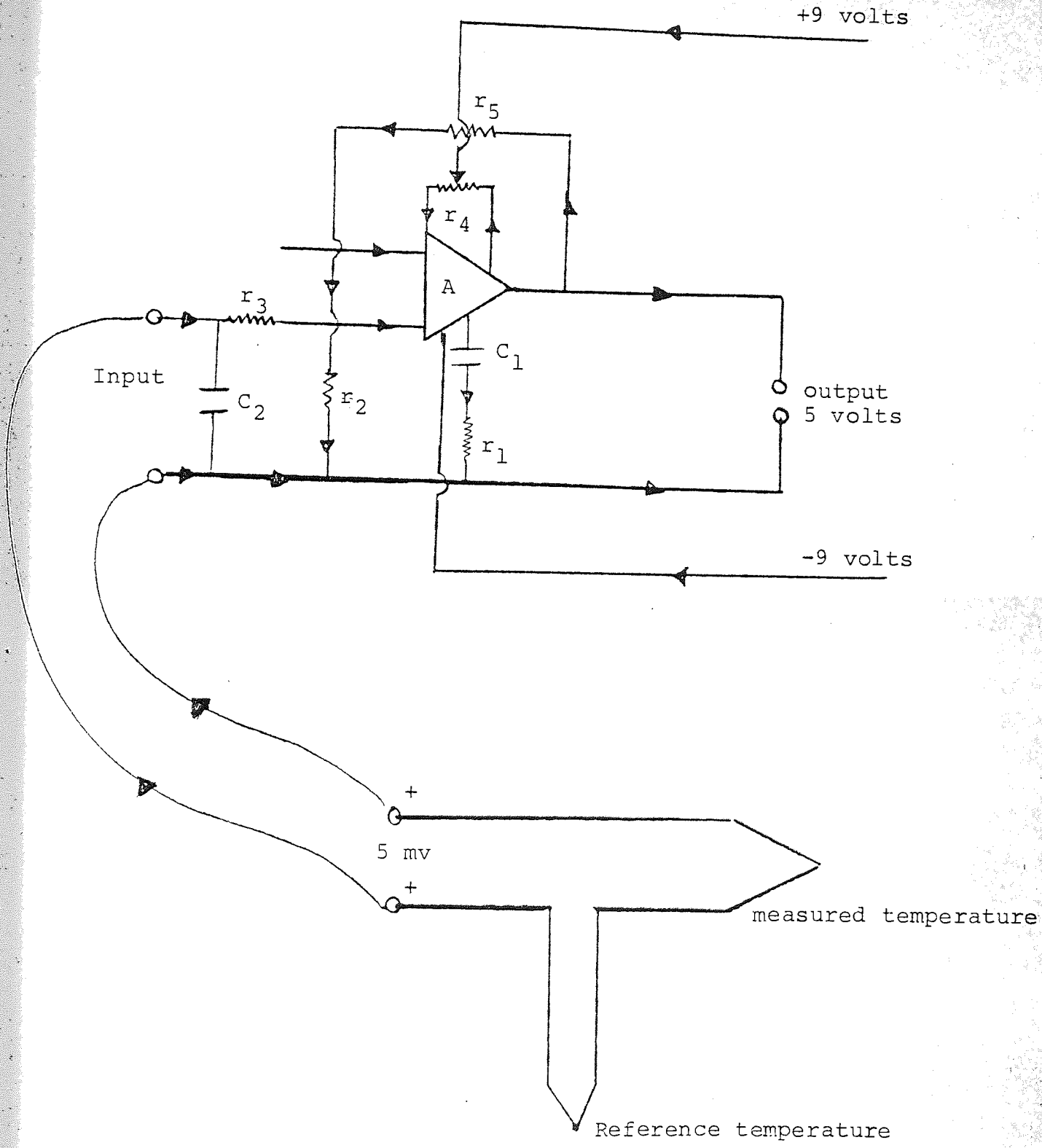
(iv) the melting point of ice as the reference temperature

(v) high capacitance capacitors of 2000 μF

(vi) a number of resistors chosen such that a gain of 1000 is obtained on the amplifier

These thermocouples have shown excellent reproducibility in calibrations with an accuracy of $\pm 0.1^{o}C$ which is comparable to the expensive zero-chamber thermocouples that are recommended for such purposes.

The characteristic equations were obtained by correlating the measured temperature to the output signal and have been tabulated in Table III.4.



Notation

A: high performance operational amplifier type 725CN
C_i: capacitors each with a capacitance of 2000 μF
r_i: resistances arranged such that the gain of 1000 is obtained on the amplifier

Figure III.4 - The Proposed Design for the Thermocouples

The characteristic curves are presented in Appendix A.3.

Thermocouple	a_i	b_i	α_i
top tray	3.81021	23.0901	.998216
feed tray	3.95769	23.0626	.9899312
bottom tray	3.63583	23.0572	.996743
feed stream	-0.307	22.1	.981326
reflux stream	4.16	20.5	.973182

Table III.4

The form of the correlations is

$$T = a + bv \quad \text{..... III.6}$$

where

T = temperature ^{o}C.

v = voltage volts

α = correlation coefficient

The curve-fittings were done by the least squares method.

III.2.2 CONTINUOUS LEVEL MEASUREMENT

The air differential pressure transducers supplied by the IBM can be used to monitor the liquid level in a vessel provided that they are isolated from the liquid by an air-lock, as demonstrated by Daie (134), in order to avoid corrosion. With such an arrangement the response of the transducer to changes of pressure, induced by the level changes in the vessel, is linear. This means that the holdup of liquid in the vessel can be correlated to the transducer output as

$$\text{Holdup} = g(\text{output voltage}) \quad \text{..... III.7}$$

The two level measurements needed for the column operation are made at the reboiler and the reflux drum. The arrangement for the reboiler is shown in Figure III.5. The arrangement for the reflux drum is similar.

The calibration and the filling-up procedures are as follow:

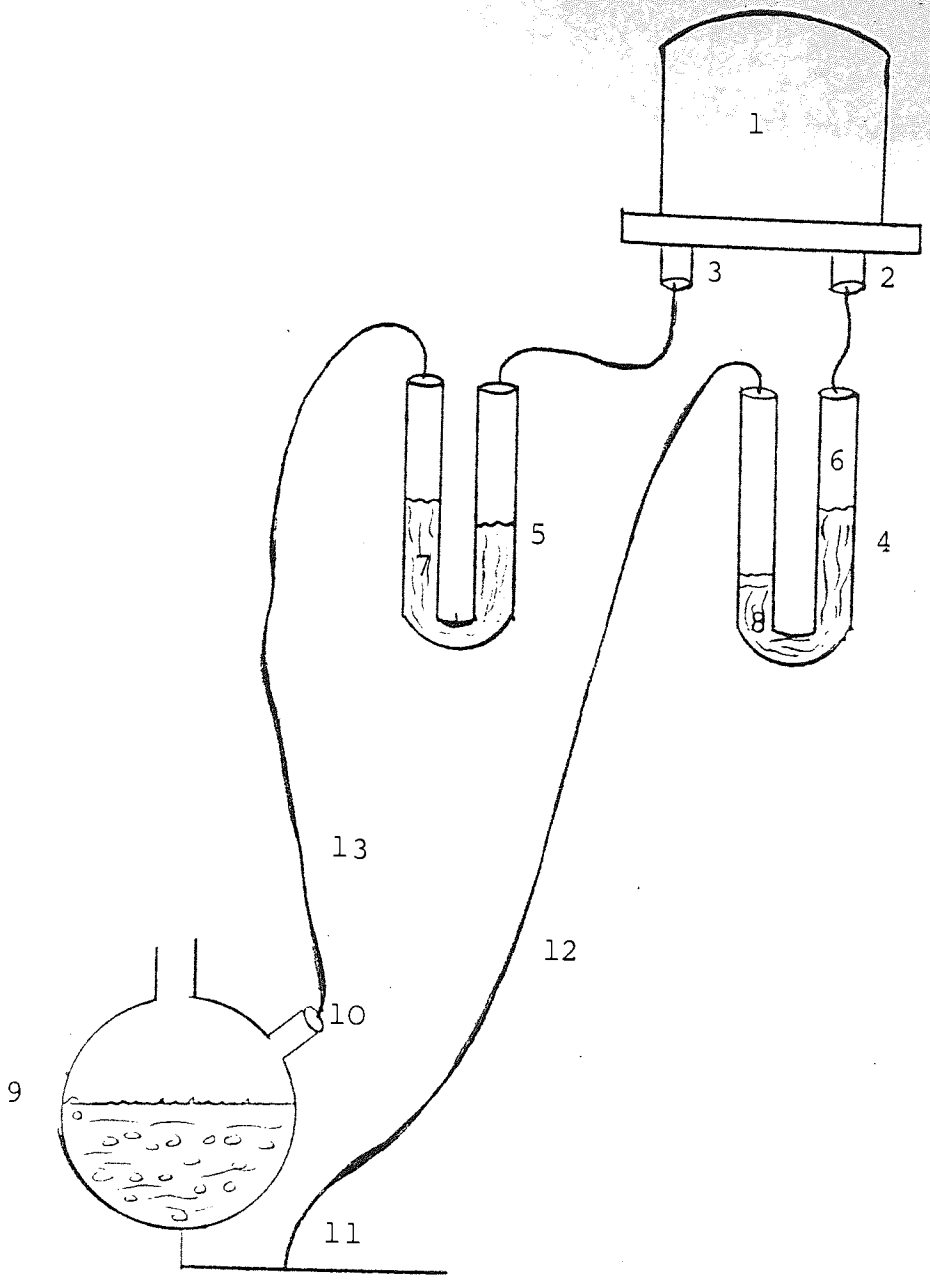
(i) empty the reboiler

(ii) disconnect the transducer connections at the transducer

(iii) place sufficient liquid in the reboiler so as to cover the dead zone in the reboiler. This can be judged visually and normally needs approximately 200 cc. of liquid

(iv) connect the upper transducer connections

(v) fill up the reboiler (in stages with known



1 : the air pressure transducer
2 : the high pressure connection
3 : the low pressure connection
4&5: the u-tubes
6 : the air-lock
7&8: water as the liquid in the u-tubes
9 : the reboiler
10&11: lower transducer connections; pressure measurement points
12&13: ¼ inch P.T.F.E. tubing

Figure III.5 - The Arrangement for the Liquid-Level Measurement in the Reboiler

masses of liquid if it is being calibrated and record the transducer reading)

The calibration of the reflux drum is simply done by inserting known masses of liquid in the drum in stages and recording the transducer output.

The calibrations are reproducible provided that the above filling-up procedure is observed. The equations describing the level indicators are:

The reboiler: $M_B = -32.9 + 23.8\ V$ III.8

The reflux drum: $M_{RD} = -0.326 + 0.513\ V$ III.9

where the holdup (M) is in kg. and the transducer reading (v) is in volts. The curve fittings were done by the least squares method.

The characteristics of the level indicators are given in Appendix A.4.

III.2.3 FLOW MEASUREMENT

In addition to measuirng the flow rate by correlating it to the valve opening, a second method could be by a similar arrangement to that of level measurement. The only difference is that the differential pressure is induced by an orifice plate instead of a difference in the liquid level. The flow rate can then be correlated to the transducer output.

The accuracy of the flow measurement by this method was found to be $\pm$50 cc./min. Although this level of accuracy may be tolerable at flow rates greater than 500 cc./min., this arrangement can be somewhat problematical at low flow rates. Due to the limitations of the maximum heat load on the reboiler, the maximum flow rate during operation had to be confined to 150 cc./min. which effectively ruled out the measurement by this method and it was not used in this research.

Nonetheless, for completeness, the calibration equations for these arrangements are given in Appendix A.4.

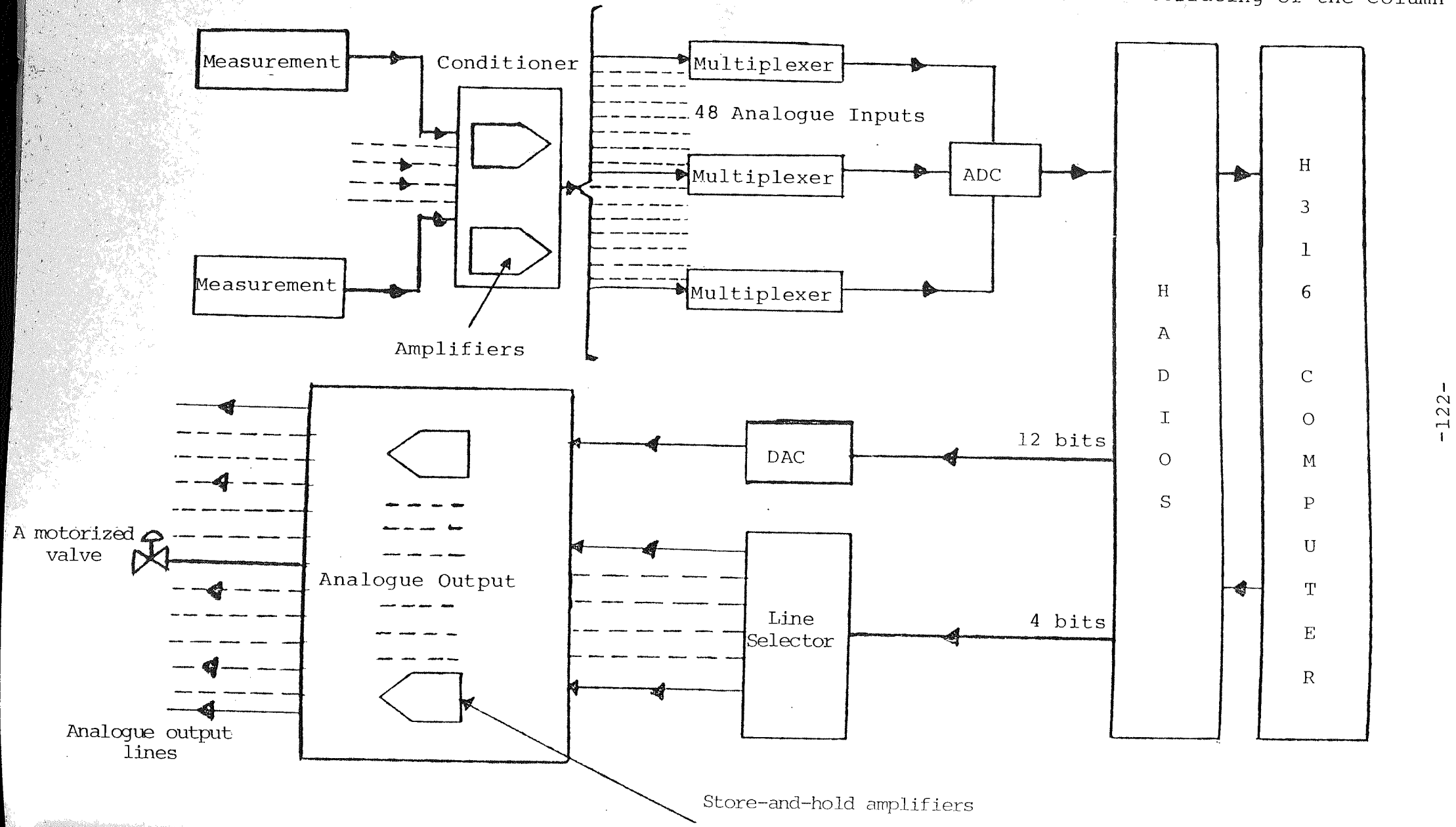
III.3 THE INTERFACING OF THE COLUMN TO THE HONEYWELL 316 COMPUTER

The hardware involved in the interfacing of the column to the Honeywell 316 computer is depicted schematically in Figure III.6. A total of 12 analogue inputs and six digital outputs are used, for data acquisition and control, on the column as it stands at present.

On the available departmental facilities, a single channel ADC is used to handle 48 analogue input channels by three multiplexers. The operation involves completing the conversion of one input, resetting the circuit and applying a new input to the converter. Thus a maximum of 48 separate analogue signals can be processed in turn by the ADC, the input signals (0 to 5v) being converted to a binary integer with a 10 bit resolution, i.e. 0 to 1023_{10}. The output devices needed for the transmission of information from the computer are mainly application dependent. As regards the distillation column this essentially comprises a line selector, a DAC and an analogue output device which comprises a series of store-and-hold amplifiers. The resolution of the DAC is 12 bits which corresponds to 0 to 10 volts.

HADIOS provides a very flexible method of interfacing the Honeywell 316 computer to a wide range input/output devices for on-line applications. It basically consists of a controller, connected to the

Figure III.6 - The Schematic Diagram of the Hardware Involved in the Interfacing of the Column



computers input/output data and control lines, which generates subsidiary data, addresses and controls for up to 15 different subinterfaces. The operation of these subinterfaces is achieved by the output of control signals (initiated by programmable command) from the computer to the HADIOS controller which then carries out the majority of address and function decoding before initiating the required function of the requested subinterface. The system also has the ability to operate under interrupt control. This kind of operation is governed by the interrupt mask circuits of the HADIOS controller which can be set by the execusion of programmable commands. The details of the programmable instructions used to operate HADIOS are given in the HADIOS manuals and also by Webb (27).

The modularity of construction of HADIOS allows systems to be simply configured to meet the particular requirements of each application. At present, the following facilities are available:

(i) 48 analogue inputs

(ii) three counters

(iii) two digital inputs

(iv) two digital outputs

Of these, only the digital outputs and analogue inputs have been employed to communicate with the present instrumentation on the column. The allocated analogue and digital channels are identified with the instrumentation on the column below in Tables III.5

and III.6 respectively.

Analogue Channel Number	Location and Function
36	Lowermost tray; thermocouple
37	Topmost tray; thermocouple
38	Feed tray; thermocouple
39	Feed flow; pressure transducer
40	Bottoms flow; pressure transducer
41	Distillate flow; pressure transducer
42	Reflux flow; pressure transducer
43	Condenser cooling water; pressure transducer
44	Reboiler LI; pressure transducer
45	Reflux drum LI; pressure transducer
46	Reflux stream; thermocouple
47	Feed stream; thermocouple

Table III.5 - The Analogue Input Channels

Digital Output Channel Number	Location and Function
A1	Reflux stream; motorized valve
A2	Bottoms; motorized valve
A3	Feed stream; motorized valve
A4	Distillate stream; motorized valve
A5	Condenser cooling water; motorized valve
A6	Reboiler

Table III.6 - The Digital Output Channels

REMOTE DATA CONDITIONING

In order to convert the signals produced by the various measuring instruments into a form compatible with HADIOS and also the signal from the computer into a form acceptable to the various electrically operated devices on the column such as the motorized valves a remote signal conditioning unit has been constructed by the departmental electricians. Within this cabinet, all the analogue signals are converted to voltages, where necessary, and then amplified into the range 0 to 5 volts D.C. Also contained in this cabinet are:

(i) the line drivers for the transmission of digital signals

(ii) the power supplies for the transducers, motorized valves and the reboiler

(iii) the analogue output device

(iii) the manual/automatic switches for the valves and the reboiler required to start up the column

This cabinet is situated adjacent to the distillation column both for convenience and also to minimize the effects of electrical noise during the transmission of signals to the computer.

III.3.1 THE HONEYWELL-316 COMPUTER

The Honeywell-316 computer is designed for both batch scientific applications and real-time on-line data processing and control. The wide variety of applications which can be implemented include data acquision, simulation, control and batch scientific computation.

These applications are undertaken using an instruction repertoire of seventy two commands, a memory cycle of 1.6 μs and input-output data handling at a maximum rate of 156 KHZ/second. The computer is a stored program, parallel binary type using two's complement machine code. A single 10-bit address with indexing and indirect addressing accesses a 16-bit (5 octal digits plus the sign bit) coincident-current ferrite core memory; one hardware index register is provided. The memory is a random access system expandable from 4k to 32k words - the computer used in this research has a memory size of 16k words. Other features of the central processing unit (cpu) include a real time clock, high speed multiply/divide and a single interrupt line.

The general characteristics of the H316 computer are given in Table III.7. The H316 computer uses the DAP-16 symbolic assembly program language for translation of source programs to mechine code. The other source program languages available to the user are FORTRAN and BASIC. The system also allows mixed-language programming.

The Peripheral Equipment

Six peripheral devices are connected to the central I/O bus of the central processor which are as follows:

(i) a high speed paper tape reader operating at 200 characters per second

(ii) a high speed paper tape punch operating at 75 characters per second

(iii) a magnetic tape cassette unit used for both input-output; input at 375 bytes per second and output at 375 bytes per second

(iv) a teletype operating at 10 characters per second

(v) a Tektronix 4010-1 visual display units (VDU). This VDU is capable of both graphical and character display and in the alphanumeric output mode operates at a rate of 200 baud. It is possible to use the VDU both in the computer room and adjacent to the distillation column. Attached to the VDU is a hard copy unit, which provides permanent copies of the display when required. The hard copy unit can be operated either by depressing a switch situated on the VDU or by programmed commands

(vi) an AED 3100p floppy disc drive unit

Primary power	475 watts, 5.5 amps. at 115 vac ± 10% at 60 ± 2HZ
Type	parallel binary solid state
Addressing	single addressing with indexing and indirect addressing
Mechine code	two's complement
Circuitry	integrated
Signal levels	active: 0 volts passive: +6 volts
Instruction complement	72 instructions
Speed, Add Subtract Multiply Divide	3.2 μs 3.2 μs 8.8 μs 17.6 μs
Standard memory	designed to protect memory data in the event of primary power failure
Standard interrupt	single standard interrupt line
Input/output modes	single word transfer single word transfer with priority interrupts
Standard I/O lines	10-bit address bus (4 function code and 6 device address); 16 input bus; 16 output bus; priority interrupt, external control and sense lines
Standard teletype	read paper tape at 10 cps; punch paper tape at 10 cps; print at 10 cps, keyboard input; off-line paper tape preparation, reproduction and listing
Environment	room ambient temperature: 0-45°C
Cooling	filtered forced air

Table III.7 - Honeywell 316 Leading Characteristics

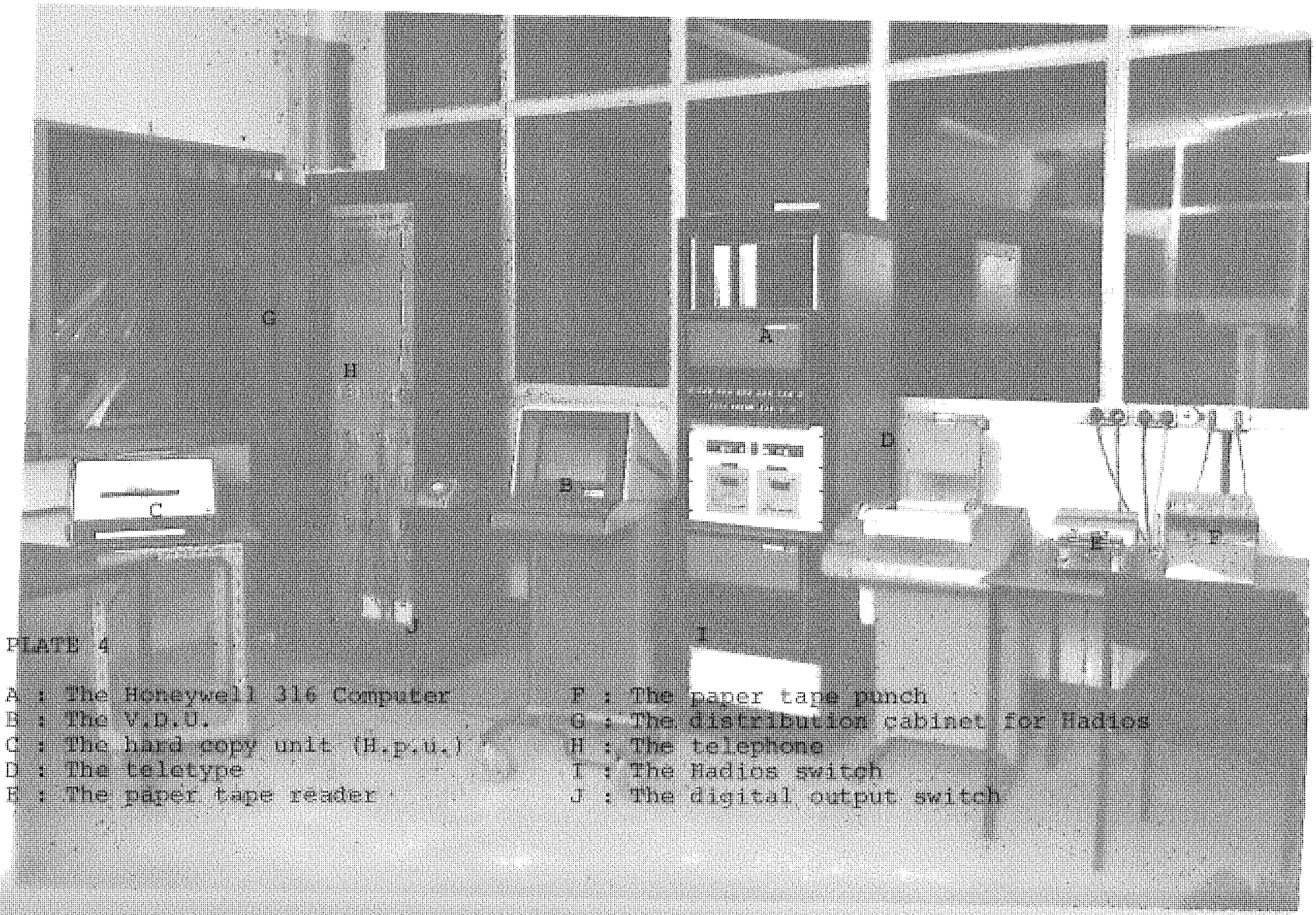


PLATE 4

A : The Honeywell 316 Computer
B : The V.D.U.
C : The hard copy unit (H.p.u.)
D : The teletype
E : The paper tape reader
F : The paper tape punch
G : The distribution cabinet for Radios
H : The telephone
I : The Radios switch
J : The digital output switch

A = the A.D.U.
B = the psrq cora
C = the telefaxe
D = the betsi fabe reseek

Houewest 3 Jo
the mif (H.b.n.)

G = the telephone
H = the aggtos awifcp
I = the qtaifsl onfbnf awifcp
J = the

III.4 PROCESS OPERATION

Start-up

The following procedure should be followed to start the column:

1. Switch the mains power on using the switch labelled MASTER on the cabinet next to the distillation columns.
2. Switch all the valves and the heater to manual mode of operation by depressing the bottons near the visual input voltage display dials.
3. Switch on
   (i) the Honeywell-316 computer and load the HADIOS Executive MOD.2
   (ii) the HADIOS : the switch labelled I on plate 4
   (iii) the digital output switch in the HADIOS distribution cabinet: the switch labelled j on plate 4
4. Empty the reboiler.
5. Recycle the feed stock a couple of times to ensure good mixing of the components.
6. Disconnect all the transducer connections at the transducers to allow air into the transducers.
7. Ensure that all the valves are working and that there are no stiction problems by closing and opening them a couple of times using the manual operation switches.

8. Fill the reboiler up to the required level by the procedure laid out in section III.2.2.
9. Connect the transducers up and check that the air-locks and the u-tubes are intact in all flow and level measurement lines.
10. Turn on the cooling water for the condenser and the heat exchange in the bottom product line.
11. Switch the heater on and run the column at total reflux for at least 20 minutes to ensure that the trays are filled (the reflux valve fully opened).

    Precaution: while operating under total reflux ensure that the manual valves preceding the feed and distillate motorized valves are fully closed.
12. Switch the feed pump on and open the feed valve gradually to allow the feed into the column.
13. Set the reflux valve to the right opening.
14. Switch the thermocouples on and switch to automatic mode of operation and let the computer take over.

The column takes approximately 30 minutes to reach steady state after which disturbances can be introduced and experimentation can begin.

Shut-down

The following shut-down procedure needs to be followed:

1. Switch the heater off.
2. Switch all pumps off.
3. Turn all the manual and motorized valves off.

4. Switch the thermocouples off.

5. Switch off the HADIOS, the H316 computer and all its associated peripherals.

6. Switch the master-switch off.

7. Allow the column to cool down for at least 30 minutes and turn off the cooling water taps.

C H A P T E R F O U R

DYNAMIC SIMULATION

IV.1 DYNAMIC SIMULATION

As processes become more complex, incorporating ever-increasing degrees of automation, there will be a greater need for the analytical approach to the problems associated with their design and operation. Deterministic analysis of multivariable systems usually involves some form of mathematical modelling which has long been a favoured preliminary to a commercial plant as far as chemical engineers are concerned. There are various mathematical models for the same system, each one suited to solve a particular problem associated with the system. Two broad classifications constitute steady-state and dynamic models, that are used for steady-state and dynamic simulations respectively.

As regards dynamic simulation, the amount of detail that needs to be included in the model is usually determined by the purpose that the dynamic simulator is to serve. For instance, a dynamic model intended for control studies may need a lesser degree of sophistication than the one geared to design and safety studies. Of interest to this thesis is the application of dynamic simulation for control studies using a digital computer and this largely governs the assumptions that are made to simplify the mathematical model of a binary distillation column to render it more practicable.

One important aspect of mathematical modelling is the arrangement of the equations. It is generally believed that if the equations are arranged in a logical

or cause-and-effect order, the computer model is stable. This sequence is normally termed as the "natural" order, for it invariably parallels the cause-and-effect sequence found in nature.

In order to avoid unnecessary duplication, "continuous digital dynamic simulation" will henceforth be referred to as simulation and, moreover, the discussion will be confined to "process simulation" using FORTRAN only.

In a simulation exercise, usually a structure is set up to encompass the mathematical model and to communicate with an integrator in order to solve the differential equations that form the mathematical model. Almost invariably the linear or non-linear differential and algebraic equations constituting the mathematical model of the system need to be solved simultaneously and thus the problem of the simultaneity of the equations must be treated with due care.

Another important issue in simulation is the problem of initialization which needs considerable care. The choice of initial conditions to solve the differential equations must be realistic and physically feasible. An unrealistic set of initial conditions can lead to divergence or a solution which, although mathematically possible, is physically nonsensical. Therefore, if physically meaningful solutions are sought, judicious choice of initial conditions is imperative.

The back-bones of a dynamic process simulator normally comprises:

(i) a definite structure for communicating with an integrator

(ii) a number of individual modules each made up from a collection of linear or non-linear algebraic and differential equations

(iii) an integrator

(iv) a channel for outputting information

(v) a library of utility routines to perform various functions such as curve fitting, arbitrary function generation, solution of non-linear algebraic equations, etc., depending on the needs of the problem.

IV.2 THE STRUCTURE OF A DYNAMIC SIMULATOR

In a dynamic process simulator next to the mathematical modelling aspects, the role of the structure relative to that of the integrator is of central importance and has considerable bearing on the flexibility of the simulator. Unfortunately, most, if not all, of the available integrators have been designed for "system" simulation and require that a structure be set up in a predefined manner to suit the integrator. The user is expected to formulate the mathematical model of the system which usually appears in the form of a subroutine that can be called by the integrator as necessary. In such structures, normally, once the integrator is called, it then takes full control of the simulation with little further user interference. In such a picture, the structure can be considered as being subordinate to the integrator. This arrangement can be somewhat limiting and cumbersome at "process" simulation level at which the simulator is, usually, expected to supply a library of individual simulator modules and the user is relieved of the mathematical modelling problems. Ideally, at process simulation level, one would like an integrator which can be called autonomously at any point within the structure to update any number of variables and report back to the structure at the end of any number of integration steps. Additionally, experience has shown that it is often helpful if the independent variable is advanced outside

the integrator as opposed to its being advanced by the integrator which is the common feature of the integrators intended for system simulation. This aspect can enhance the flexibility of the integrator, and hence that of the simulator, in the following ways:

(i) it enables frequent step size and integration order manipulations to achieve superior computational efficiency

(ii) it enables different control and estimation routines to be interlocked into the simulator with relatively more ease and without having to restructure the simulator modules

(iii) in on-line application and when variable step integration methods are being used, the chances of missing a sample or a control point can easily be made zero with little programming effort.

In other words, the integrator is subordinate to almost any structure that may be fit for a certain problem. To bring this about, a collection of four FORTRAN subroutines, namely, SDINT, INTJS, INTPAS and PRINT are proposed. These will be henceforth referred to as the SDINT subroutines.

Experience with a wide range of typical chemical engineering problems has shown that, with almost no exception, the fourth-order Runge-Kutta method is quite adequate for any situation and that the second- and first-order methods will provide reasonable accuracy coupled with greater computational speed. The SDINT subroutines offer a choice of three different fixed

step integration methods which are as follows:

(i) the Euler's method; a first order method

(ii) the Euler's predictor-corrector method; a second order method

(iii) the fourth-order Runge-Kutta method; a fourth order method

Due to the important role of the integrator in any dynamic simulation study some elaboration on the general arrangement of the main program and that of the individual simulator modules will be in order at this stage. The full documentation of the SDINT subroutines is given in Appendix B. A simple example of how the SDINT subroutines can be used to simulate a system is also given in Appendix B. The system chosen for illustration is described by a second order ordinary differential equation that is reduced to a set of two first order differential equations which must be solved simultaneously.

General Arrangement of the Main Program for the Use of the SDINT Subroutines

The main programme arrangement is depicted in Figure IV.1. Following a preliminary housekeeping section containing FORMATS and DECLARATION statements, the initialization section is laid out. Here all the calculations and specifications for the problem parameters and coefficients are made. These are the values that are normally invariant during the course of the

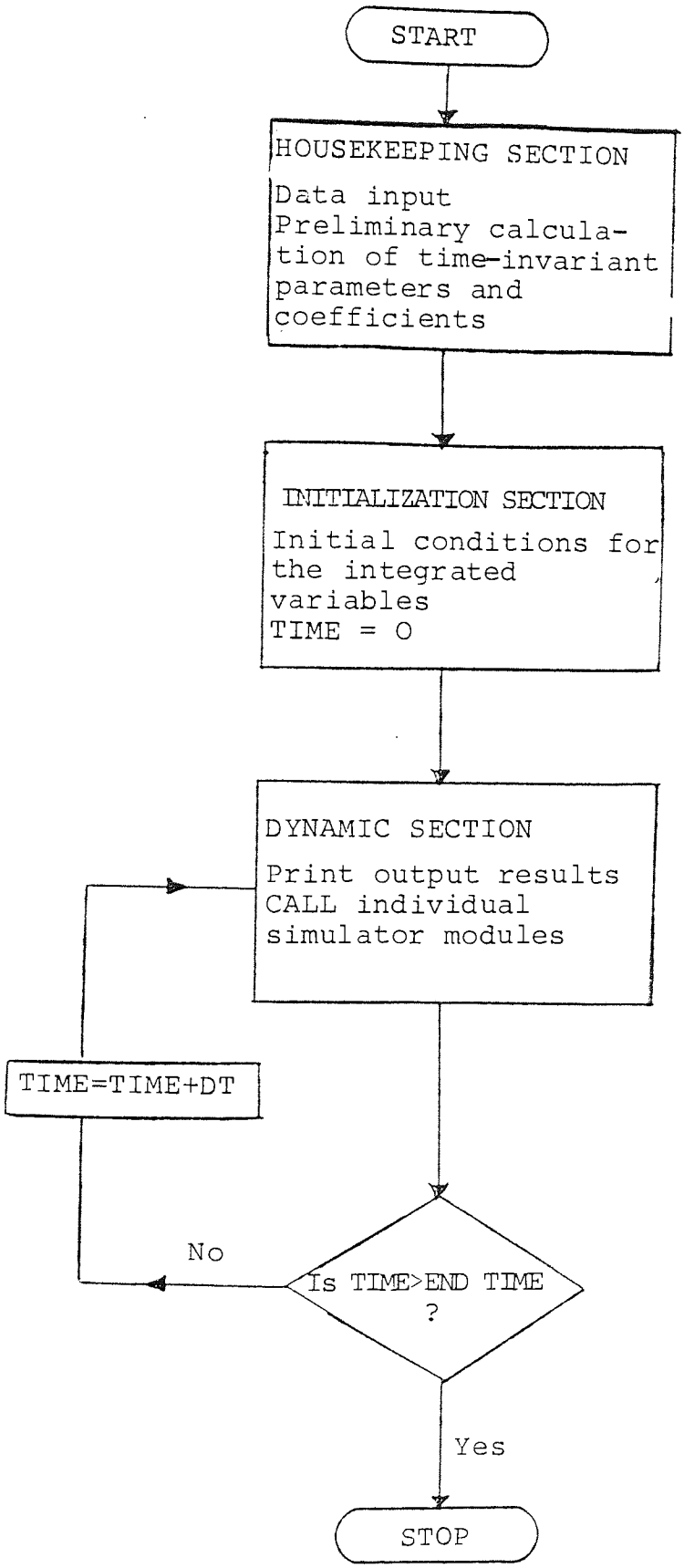


Figure IV.1 General Arrangement of the Main Program for the Use of SDINT Subroutines.
DT Is the Integration Step Size.

calculations. In this section the initial conditions for the integrated variables must also be specified and the independent variable must be set to zero. The next section is the dynamic section in which the individual simulator modules are called to perform the simulation and the independent variable is advanced when all the modules have been updated.

The Program Arrangement for the Individual Simulator Modules

The individual simulator modules must be laid out according to the flowchart shown in Figure IV.2. Each module essentially comprises:

(i) the preliminary calculation section (if necessary)

(ii) the derivative section in which the derivatives are computed

(iii) the integration section where the integrated variables are updated

(iv) the test for the step completion and a CALL to the subroutine INTPAS to zero the integrator pass numbers for the next integration step.

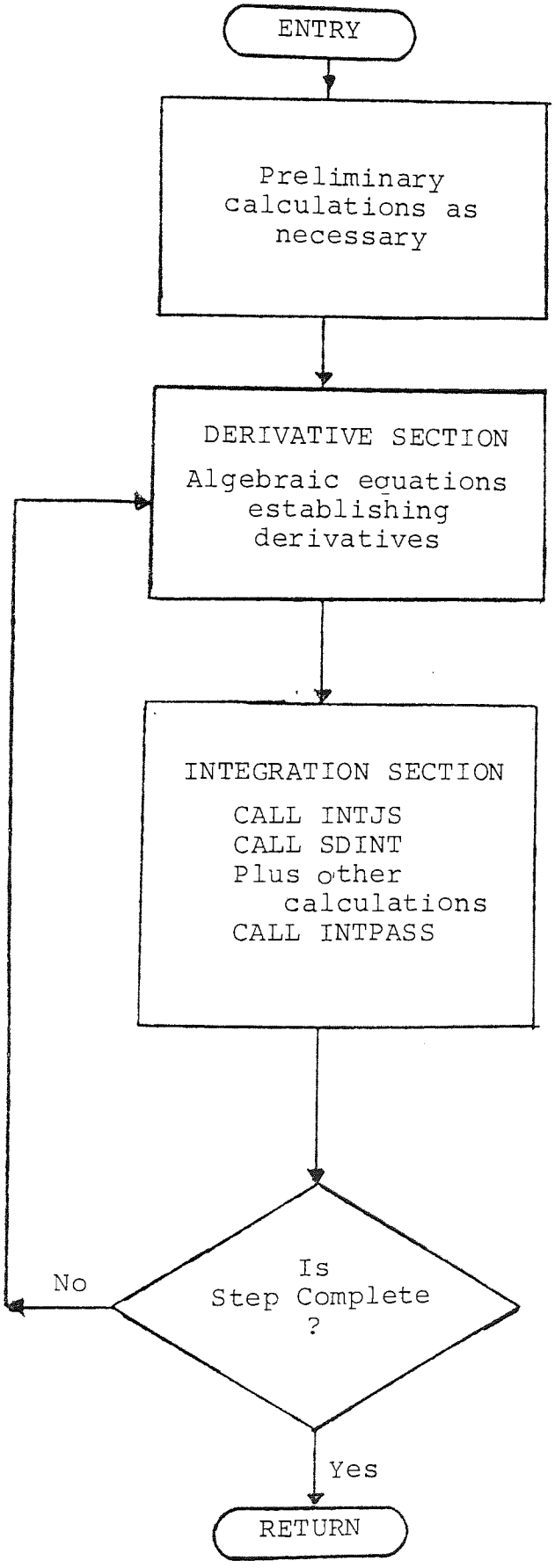


Figure IV.2 Subprogram Arrangement for a Simulator Module

IV.3 MATHEMATICAL MODEL OF A DISTILLATION COLUMN

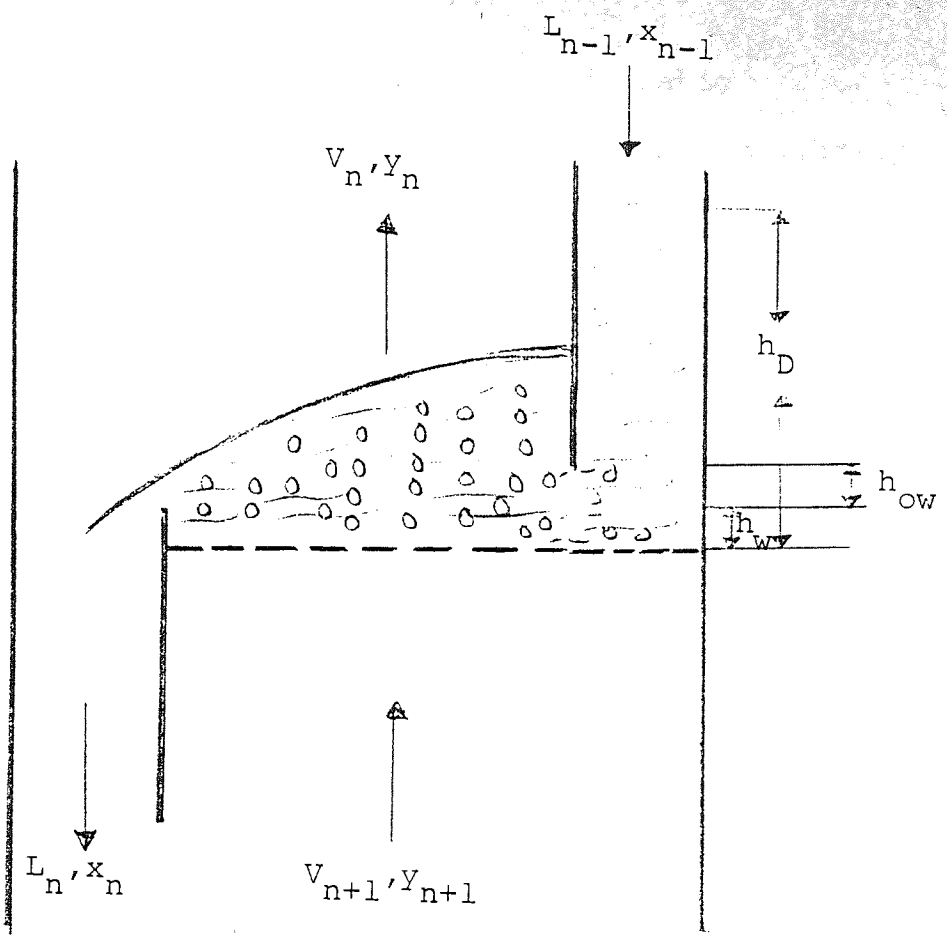
The model of a distillation column can be approximated by modelling a typical tray with ideal vapour-liquid equilibrium and stepping this up from a single tray to a column with a number of similar trays. The models of the column accessaries such as the reboiler and the condenser can then be added to this picture to enable a complete mathematical description of the column. Further sophistications such as allowing for the non-ideality of the vapour-liquid equilibrium and real trays can then be introduced as necessary.

As indicated before, the perfectly mixed tray model is not only more flexible but also amenable to solution by digital computers and thus it will be adopted for the modelling of a tray in this thesis.

IV.3.1 THE MATHEMATICAL MODEL OF A TYPICAL TRAY

A typical tray is depicted in Figure IV.3. The assumptions that are made in its modelling are as follows:

1. Liquid on the tray is perfectly mixed and incompressible
2. The time constants for the fluid and thermal transfers are negligible compared with that for the mass transfer
3. Vapour hold-up is negligible compared with liquid hold-up



h_D = liquid height in the downcomer

h_{ow} = liquid height over the weir

h_w = height of the weir

M_L = liquid hold-up

L_n, V_n = liquid and vapour flow rates respectively

Figure IV.3 The Schematic Diagram of a Typical Tray

4. The column is essentially adiabatic

5. Vapour and liquid are in thermal equilibrium, i.e. at the same temperature, but not in phase equilibrium. A Murphree vapour-phase efficiency will be used to describe the departure from the equilibrium.

It is assumed that n denotes the plate number and j refers to the number of components.

(i) total continuity equation : one per tray

$$\frac{d}{dt}(M_n) = (L_{n-1}+V_{n+1}) - (L_n+V_n) \quad \ldots\ldots\ldots \text{IV.1}$$

(ii) component continuity equation : J-1 per tray

$$\frac{d}{dt}(M_n x_n) = (L_{n-1}x_{n-1}+V_{n+1}y_{n+1}) - (L_n x_n+V_n y_n) \quad \ldots\ldots\ldots \text{IV.2}$$

(iii) energy equation : one per tray

$$\frac{d}{dt}(M_n U_n) = (L_{n-1}h_{n-1}+V_{n+1}H_{n+1}) - (L_n h_n+V_n H_n) \quad \ldots\ldots\ldots \text{IV.3}$$

where

M_n = molar liquid hold-up

x_n = liquid composition on the nth tray (mole fraction)

y_n = vapour composition on the nth tray (mole fraction)

U_n = the internal energy (kJ/mol)

h_n = liquid enthalpy (kJ/mol)

L_n = liquid rate from the nth tray (mol/hr)

V_n = vapour rate from the nth tray (mol/hr)

(iv) phase equilibrium : J per tray

$$y_n^* = g(f_n, x_n, T_n, \gamma_n) \quad \text{..... IV.4}$$

where

y_n^* = vapour composition in equilibrium with x_n

f_n = fugacity (atm.)

T_n = bubble point temperature ^{o}C.

γ_n = activity coefficient

(v) fluid dynamic relationships:

(a) liquid; one per tray

with reference to Figure IV.3 we have:

$M_{L,n} = f(h_w, h_{ow}, h_D,$ hydraulic gradient across the tray, time) IV.5

The exact relationship between liquid hold-up and liquid flow rate would be too complex if commonly used correlations for each liquid head term were evaluated. However, a commonly used expression is that of Brambilla (110) which is of the form:

$$M_{L,n} = A + BL_n + CF_n + Dh_w \quad \text{..... IV.6}$$

where

F = vapour flow parameter = (vapour density)$^{.5}$(vapour velocity)

A,B,C and D = constants available for different types of plates

(b) vapour; one per tray

$$V_n = f(P_n, P_{n+1}, y_{n,j}, T_n) \quad \text{..... IV.7}$$

This equation is usually of the form

$$V_n^2 = \frac{P_{n+1} - P_n}{K_{DP} \cdot \zeta_n^v}$$

where ζ_n^v is the vapour density on the nth tray and K_{DP} is the pressure-drop coefficient.

(vi) actual vapour composition equations; j per tray

$$Y_{n,j} = Y_{n+1,j} + E_{n,j}(y^*_{n,j} - y_{n+1,j}) \quad \text{..... IV.8}$$

whre $E_{n,j}$ denotes the Murphree vapour-phase efficiency and * denotes the equilibrium value.

(vii) thermal properties; two per plate

$$h_n = f(x_{n,j}, T_n)$$
$$H_n = f(y_{n,j}, T_n, P_n) \quad \text{..... IV.9}$$

IV.4 THE MODEL OF A BINARY DISTILLATION COLUMN

Most columns, in actuality, handle multicomponent feeds. But many can be approximated by binary or pseudo-binary mixtures. Therefore, binary distillation columns assume a very important position in the chemical plants. The objective here is to derive the mathematical model of a conventional binary distillation column with a total condenser and a reboiler and explore the possibility of making further simplifying assumptions to render the solution more practicable. The schematic diagram of the column is given in Figure IV.4.

IV.4.1 MODEL I

The purpose of studying this simplified case is to reduce the problem to its most elementary form so that the basic structure of the equations can be clearly seen. The following additional assumptions are made in the formulation of this model:

(i) the feed and reflux streams enter the column as saturated liquids at their bubble points

(ii) constant column pressure

(iii) equimolal overflow, i.e. $V_{n-1}=V_n=V_{n+1}=V$

(iv) negligible time lags in the reboiler and condenser responses.

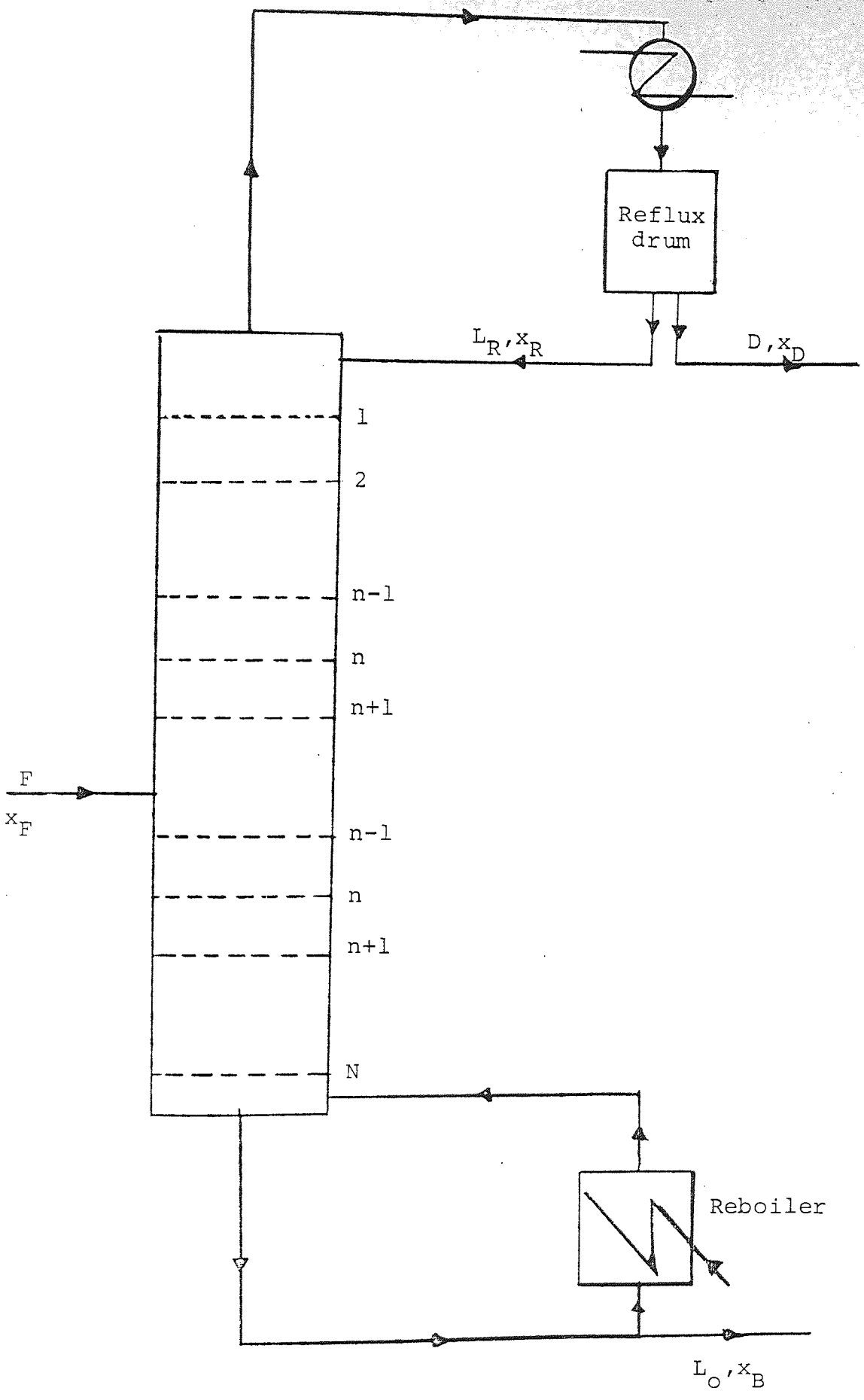


Figure IV.4 Schematic Diagram of a Conventional Distillation Column with a Total Condenser

(a) The Model of a Typical Tray

Total continuity: $$\frac{d}{dt} M_n = L_{n-1} - L_n \quad \ldots\ \text{IV.10}$$

Component continuity: $$\frac{d}{dt} (M_n x_n) = L_{n-1} x_{n-1} + V y_{n+1} - L_n x_n - V y_n \quad \ldots\ \text{IV.11}$$

for the most volatile component (M.V.C.)

Differentiating IV.11 and substituting for $\frac{d}{dt} M_n$ from IV.10, equation IV.11 can be rearranged into the form

$$M_n \frac{d}{dt} x_n = L_{n-1}(x_{n-1} - x_n) + V(y_{n+1} - y_n) \quad \ldots\ \text{IV.12}$$

Fluid dynamic equation: $$L_n = \frac{M_n - A}{B} \quad \ldots\ \text{IV.13}$$

Vapour-liquid equilibrium: $$y_n^* = f(x_n, T_n, P) \quad \text{IV.14}$$

for the M.V.C.

Where P is the total column pressure and T_n is the bubble point temperature.

Actual vapour composition calculation: $$y_n = y_{n+1} + E_n (y_n^* - y_{n+1}) \quad \ldots\ \text{IV.15}$$

(b) The Model of the Feed Tray

Total continuity: $$\frac{d}{dt} M_n = L_{n-1} - L_n + F \quad \ldots\ \text{IV.16}$$

Component continuity for the M.V.C.: $$M_n \frac{d}{dt} x_n = L_{n-1}(x_{n-1} - x_n) + V(y_{n+1} - y_n) + F(x_F - x_n) \quad \ldots\ \text{IV.17}$$

Fluid dynamic equation: $$L_n = \frac{M_n - A}{B}$$

..... IV.18

Vapour-liquid equilibrium: $$y_n^* = f(x_n, T_n, P)$$

..... IV.19

Actual vapour composition: $$y_n = y_{n+1} + E_n(y_n^* - y_{n+1})$$

calculation IV.20

(c) The Model of the Reboiler

Total continuity: $$\frac{d}{dt} M_n = L_{n-1} - L_o - V$$

..... IV.21

where; L_o = the bottoms rate

Component continuity: $$M_n \frac{d}{dt} x_n = L_{n-1}(x_{n-1} - x_n) + V(x_n - y_n)$$

for the M.V.C.

..... IV.22

Energy equation: $$V = \frac{Q}{\lambda}$$

..... IV.24

where Q = the heat duty kJ/hr.

λ = the average latent heat kJ/mol.

Vapour-liquid equilibrium: $$y_n^* = f(x_n, T_n, P)$$

for the M.V.C. IV.24

Actual vapour composition: $$y_n = x_n + E_n(y_n^* - x_n)$$

..... IV.26

(d) The Model of the Condenser and Reflux Drum

Total Continuity: $\frac{d}{dt} M_D = V - L_R - D$

..... IV.27

where; L_R = the reflux rate

D = the distillate rate

Component continuity: $M_D \frac{d}{dt} x_D = V(y_1 - x_D)$

for the M.V.C. IV.28

where; x_D = the reflux composition

y_1 = vapour composition leaving the topmost plate

IV.4.2 MODEL II : a More Comprehensive Model

The assumptions of equimolal overflow and the feed and reflux streams entering the column at their bubble points which were made in the derivation of the previous model for binary distillation columns appear to be somewhat idealised and unrealistic. Model II eliminates these two assumptions by making an energy balance across each tray. With reference to Figure III.3 the following energy balance was written in section III.3.1.

$$\frac{d}{dt}(M_n U_n) = (L_{n-1}h_{n-1}+V_{n+1}H_{n+1}) - (L_n h_n+V_n H_n) \quad . \text{IV.24}$$

where U is the internal energy term and the rest of the symbols are as defined before.

The accumulation term, $\frac{d}{dt}(M_n U_n)$, is negligible compared with the heat fluxes through the tray and can be eliminated. This effectively means that one is assuming quasi steady-state conditions which will yield the following equation for the calculation of the vapour rate leaving each tray:

$$V_n = \frac{L_{n-1}h_{n-1} + V_{n+1}H_{n+1} - L_n h_n}{H_n} \quad \ldots\ldots\ldots \text{IV.30}$$

where: $h_n = \Sigma h_j x_j$

$$H_n = \Sigma H_j y_j$$

$$h_j = \int_{T^o}^{T} C_{p,j}.dT$$

$$H_j = h_j + \lambda_j$$

where: T^{o} = a reference temperature

λ_j = the latent heat of vaporization of the jth component

and the rest of the symbols are as defined before.

This approach also enables us to allow for the sub-cooling of the feed and reflux streams. Thus, using this equation the binary distillation column model can be formulated more accurately as follows:

(a) The Model of a Typical Tray

Total continuity: $\frac{d}{dt} M_n = (L_{n-1} L_n) + (V_{n+1} - V_n)$

..... IV.31

Component continuity: $M_n \frac{d}{dt} x_n = L_{n-1}(x_{n-1} - x_n)$

for the M.V.C. $+ V_n(x_n - y_n) + V_{n+1}(y_{n+1} - x_n)$

..... IV.32

Energy equation: $V_n = \frac{L_{n-1}h_{n-1} + V_{n+1}H_{n+1} - L_n h_n}{H_n}$

..... IV.33

Fluid dynamic equation: $L_n = \frac{M_n - A}{B}$

..... IV.34

Vapour-liquid equilibrium: $y_n^* = f(x_n, T_n, P)$

for the M.V.C. IV.35

Actual vapour composition: $y_n = y_{n+1} + E_n(y_n^* - y_{n+1})$

calculation IV.37

(b) The Model of the Feed Tray

Total continuity: $\frac{d}{dt} M_n = (L_{n-1}-L_n) + (V_{n+1}-V_n) + F$

..... IV.37

Component continuity: $M_n \frac{d}{dt} x_n = L_{n-1}(x_{n-1}-x_n) + V_n(x_n-y_n)$

for the M.V.C. $+ V_{n+1}(y_{n+1}-x_n) + F(x_F-x_n)$

..... IV.35

where F and x_F are the feed rate and composition respectively.

Energy balance equation: $V_n = \frac{L_{n-1}h_{n-1}+V_{n+1}H_{n+1}-L_nh_n+Q_F}{H_n}$

..... IV.39

where; $Q_F = F \Sigma q_j x_j$

and $q_j = C_{P,j}(T_F-T^O)$

T_F = the feed temperature

T^O = a reference temperature

Fluid dynamic equation: $L_n = \frac{M_n - A}{B}$

..... IV.40

Vapour-liquid equilibrium: $y_n^* = f(x_n, T_n, P)$

for the M.V.C. IV.41

Actual vapour composition: $y_n = y_{n+1} + E_n(y_n^*-y_{n+1})$

calculation IV.42

(c) The Model of the Reboiler

Total continuity: $$\frac{d}{dt} M_n = (L_{n-1}-L_o)-V_n \quad \text{..... IV.43}$$

Component continuity for the M.V.C.: $$M_n \frac{d}{dt} x_n = L_{n-1}(x_{n-1}-x_n) + V_n(x_n-y_n) \quad \text{..... IV.44}$$

Energy equation: $$V_n = \frac{L_{n-1}h_{n-1}-L_o h_o+Q}{H_n} \quad \text{..... IV.45}$$

Fluid dynamic equation: $$L_n = \frac{M_n-A}{B} \quad \text{..... IV.46}$$

Vapour-liquid equation for the M.V.C.: $$y_n^* = f(x_n,T_n,P) \quad \text{..... IV.47}$$

Actual vapour composition calculation: $$y_n = x_n+E_n(y_n^*-x_n) \quad \text{..... IV.48}$$

(d) The Model of the Condenser and Reflux Drum

Total continuity: $$\frac{d}{dt} M_D = V_1-L_R-D \quad \text{..... IV.49}$$

Component continuity: $$M_D \frac{dx_D}{dt} = V_1(y_1-x_D) \quad \text{..... IV.50}$$

IV.4.3 TRAY EFFICIENCY

The efficiency of a tray for mass transfer depends upon three sets of design parameters:

1. The system to be separated - its composition and properties
2. Flow conditions - rates of throughput
3. Geometry - tray type and dimensions

In arriving at a value for tray efficiency, one may rely upon plant test data or on judicious use of pilot-plant efficiency measurements. If such direct information is not available, one must resort to the predictive methods.

Methods for predicting tray efficiency are of two general types:

1. Empirical or statistical methods
2. Theoretical or semi-theoretical mass transfer methods

The first method lumps the individual tray efficiencies together and thus gives the overall column efficiency (1). The second involves the prediction of individual tray efficiencies which is of more interest to dynamic simulation of tray distillation columns.

Theoretical Predictive Methods

The approach to equilibrium on a tray may be

defined as the ratio of the actual change in vapour composition as it passes through the tray to the change that would have occurred if the vapour had reached a state of equilibrium with the liquid. If a point on plate n is considered, this definition leads to the point efficiency:

$$E_{OV} = \left(\frac{y_n - y_{n+1}}{y_n^* - y_{n+1}}\right)_{point} \quad \text{..... IV.51}$$

where y_n^* is the vapour concentration in equilibrium with the liquid concentration at the point. This efficiency cannot exceed 1 (100 percent). If there are liquid-concentration gradients on the tray, i.e. the tray liquid is not completely mixed, then y* will vary and E_{OV} may vary from point to point on the tray. It should be noted that an analogous efficiency expression could also be expressed on the basis of liquid concentrations. Equally well, vaporization efficiency as defined by Holland (111) could be used:

$$E_V = \frac{y_n}{y_n^*} \quad \text{..... IV.52}$$

For the entire tray, and for vapour concentrations, the Murphree vapour efficiency is defined as follows:

$$E_{MV} = \left(\frac{y_n - y_{n+1}}{y_n^* - y_{n+1}}\right)_{plate} \quad \text{..... IV.53}$$

where y_n^* is the vapour concentration in equilibrium with the concentration of the liquid leaving the plate. Because of concentration gradients E_{MV} can exceed 100 percent.

The best established method for predicting E_{MV} is that of A.I.Ch.E. (112). It was originally developed for binary mixtures on bubble cap trays and was later extended to other types of trays (115). It is based on the sequential prediction of point efficiency, murphree plate efficiency and hence the overall column efficiency:

$$E_{OV} \longrightarrow E_{MV} \longrightarrow E_{OC}$$

On the basis of the two film model for mass transfer and relating the efficiencies to the vapour phase concentrations, the point efficiency can be expressed in terms of mass transfer units as:

$$E_{OV} = 1 - \exp(-N_{OV}) \quad \text{..... IV.54}$$

where N_{OV} is the overall mass transfer units which can be calculated from:

$$N_{OV} = \frac{1}{\frac{1}{N_V} + \frac{\lambda}{N_\ell}} \quad \text{..... IV.55}$$

where: N_V = vapour-phase transfer units

N_ℓ = liquid-phase transfer units

λ = stripping factor which is given by $\frac{mV_m}{L_m}$

m = the slope of the equilibrium curve

V_m = molar vapour rate, moles/hr.

L_m = molar liquid rate, moles/hr.

Therefore, the evaluation of point efficiencies reduces to the prediction of the point values of N_V and N_ℓ, plus the evaluation of m, V_m and L_m for the particular

conditions under investigation.

For distillation separations, most of the resistance to mass transfer occurs in the vapour phase and therefore the calculation of N_V assumes primary importance in efficiency prediction. The A.I.Ch.E. work correlates N_V as follows:

$$N_V = \frac{0.776 + 0.116h_w - 0.290U_a\zeta_v^{0.5} + 0.0217W}{N_{scg}^{0.5}} \quad \text{..... IV.56}$$

where:

h_w = weir height in.

U_a = vapour velocity through the active area ft/sec.

W = liquid flow rate, gal./min.-ft. of the width of the flow path on the plate

N_{scg} = vapour-phase Schmidt number: given by $\frac{\mu_V}{\zeta_V D_V}$

where

μ_V, ζ_V and D_V are the vapour-phase viscosity, density and diffusivity respectively.

The liquid-phase transfer units may be obtained from:

$$N_\ell = k_\ell a \theta_\ell \quad \text{..... IV.57}$$

where

k_ℓ = liquid-phase transfer coefficient ft/sec.

a = effective interfacial area for mass transfer, sq.ft./cu.ft. of the froth on the tray

θ_ℓ = residence time of liquid in the froth zone sec.

The froth zone represents a volume with base equal to the active area of the tray and height h_f equal to the froth level that would be observed through a window for viewing contacting action on the tray. In the absence of visual observations, h_f can be calculated from the A.I.Ch.E. equation:

$$h_f = 2.53U_a^2\zeta_v + 1.89h_w - 1.6 \quad \text{..... IV.58}$$

where:

h_f	= froth height	in.
U_a	= linear vapour velocity through the active area	ft/sec.
ζ_v	= vapour density	lb/cu.ft.
h_w	= weir height	in.

Thus the liquid residence time is

$$\theta_\ell = \frac{h_f A_a \phi_t}{12q} \quad \text{..... IV.59}$$

and since the average relative froth density on the tray, ϕ_t, is equal to $\frac{h_\ell}{h_f}$,

$$\theta_\ell = \frac{h_\ell A_a}{12q} \quad \text{..... IV.60}$$

where:

q	= liquid flow rate	cu.ft/sec.
A_a	= active area	sq.ft.
h_ℓ	= pressure drop through the aerated liquid	in.
	$= \beta h_{ds}$	
h_{ds}	= calculated height of clear liquid over the disperser	in.
β	= aeration factor calculated from a correlation given by Perry(1)	

For sieve plates:

$$h_{ds} = h_w + h_{ow} + \frac{h_{hg}}{2} \quad \text{..... IV.61}$$

where:

h_w = weir height in.

h_{ow} = height of the liquid over the weir (inches of clear liquid)

h_{hg} = hydraulic gradient across the plate (inches of clear liquid)

where the height of the liquid over the wier may be calculated from the Francis weir equation (1).

The mass-transfer coefficient of equation IV.57 is carried as a product with the interfacial area to give a volumetric mass-tranfser coefficient:

$$K_l a = (1.065 \times 10^{4} D_l)^{0.5} (0.26 U_a \zeta_v^{0.5} + .15) \quad \text{..... IV.62}$$

where D_l is the liquid diffusion coefficient in sq.ft./hr. The rest of the symbols are as defined before.

As noted before, because of incomplete mixing, it is necessary in most instances to convert the point efficiency E_{OV} to Murphree plate efficiency E_{MV}, since only in small laboratory columns and under special conditions is the assumption $E_{OV} = E_{MV}$ likely to be valid. The A.I.Ch.E. method suggests an eddy diffusion model to convert point efficiency to Murphree plate efficiency. According to this model,

$$\frac{E_{MV}}{E_{OV}} = \frac{1-\exp(-n'-N_{pe})}{(n'+N_{pe})\{1+\frac{n'+N_{pe}}{n'}\}} + \frac{\exp(n')-1}{n'\{1+\frac{n}{n'+N_{pe}}\}} \quad \text{..... IV.63}$$

where

$$n' = \frac{N_{pe}}{2}\left(\sqrt{1+4\lambda\frac{E_{OV}}{N_{pe}}} - 1\right)$$

N_{pe} = peclet number = $\frac{Z^2_\ell}{D_E\theta_\ell}$

Z_ℓ = length of the liquid travel ft.

λ = stripping factor

D_E = eddy diffusion coefficient sq.ft/hr.

The value of θ_ℓ can be calculated from equation IV.60. The term D_E is an eddy diffusion coefficient. For bubble-cap trays it may be obtained from

$$D_E^{0.5} = 0.0124 + 0.0171U_a + 0.0025\frac{q'}{w} + 0.015h_w \quad \ldots\ldots\ldots \text{IV.64}$$

where

q' = liquid flow rate gal/min.

w = width of the flow path ft.

$= \frac{d_C+d_i}{2}$

d_C and d_i = column and liquid inlet diameter

For sieve trays it is suggested that the values of D_E obtained from equation IV.64 should be multiplied by 1.25 (1).

The effect of entrainment has not been considered since most columns normally operate in the region of minimum entrainment.

From a computational viewpoint, if individual efficiencies are evaluated independently, the A.I.Ch.E. method may lead to further problems in the calculation of vapour phase compositions. For example, the sum of the calculated vapour phase mole fractions may not

add to unity. This problem can be overcome by calculating the mole fraction of one of the components by difference as:

$$y_i = 1 - \sum_{i+1}^{j} y_k \quad \text{..... IV.65}$$

According to the physical properties of the components of a system, the point efficiency may be related to only one of the vapour or the liquid transfer units. In equation IV.55, one of the values of $\frac{1}{N_v}$ or $\frac{\lambda}{N_\ell}$ may be much larger than the other. If $\frac{1}{N_v}$ is much larger than $\frac{\lambda}{N_\ell}$, the value of $\frac{\lambda}{N_\ell}$ becomes negligible and may be ignored. Such a system is controlled by the vapour phase resistance. If the opposite is true then $\frac{1}{N_v}$ can be ignored. Such a system is defined as liquid film controlling. The determination of the controlling film element is affected by the value of the stripping factor, λ, which is a direct function of the slope of the equilibrium curve. For a system with a flat equilibrium curve, λ may be very small and thus $\frac{\lambda}{N_\ell}$ may be ignored giving a vapour film controlled system. On the other hand, the liquid systems with a steep equilibrium curve usually yield a liquid film controlling system.

IV.4.4 EFFICIENCY OF THE REBOILER

The form of the equation known as the vaporization efficiency is obtained by application of the Murphree efficiency to the reboiler stage. The value of y_{n+1} will be zoro in equation IV.53 since no vapour is entering the stage. Unless some experimental values of vaporization efficiency are available, the application of this efficiency definition will result in the further problem of evaluating the vaporization efficiency. It was therefore decided to use the following efficiency definition for the reboiler as suggested by Dilfanian (115):

$$E_{OV} = \left(\frac{y_n - x_n}{y_n^* - x_n}\right)_{\text{reboiler}} \quad \text{..... IV.66}$$

IV.4.5 PHASE EQUILIBRIA

Thermodynamics of Vapour-liquid Equilibrium

Thermodynamic equilibrium is defined as the final point of a reversible process and from this definition the condition of equilibrium can be expressed mathematically. Thus if a system were at its equilibrium state, there would be no change in its pressure, temperature and conditions. Moreover, the change in free energy, work, heat and entropy of the system under equilibrium would be zero.

Making the usual assumptions, it can be shown (113,122), that the fundamental equation of phase equilibrium can be written as:

$$f_i^L = f_i^V \quad \text{..... IV.67}$$

where f refers to the fugacity and L and V refer to the liquid and vapour phases respectively.

Equation IV.67 is of little practical use unless the fugacities can be related to experimentally accessible qualities x, y, T and P where x and y stand for the mole fractions of liquid and vapour phases respectively. P is the total pressure of the system which is assumed to be the same for both phases and T is the absolute temperature. The desired relationship between fugacities and experimentally accessible quantities is facilitated by two auxiliary functions which are given the symbols ψ and γ. The first of these, the fugacity coefficient ψ relates the vapour-phase fugacity f_i^V to the mole fraction y_i, and the total pressure P. It is defined by

$$\psi_i = \frac{f_i^V}{y_i P} \quad \text{..... IV.68}$$

The activity coefficient γ relates the liquid-phase fugacity f_i^L to the mole fraction x_i and to a standard state fugacity f_i^{OL}. It is defined by

$$\gamma_i = \frac{f_i^L}{x_i f_i^{OL}} \quad \text{..... IV.64}$$

From equations IV.67, IV.68 and IV.69 the equilibrium equation for any component i becomes

$$\psi_i y_i P = \gamma_i x_i f_i^{OL} \quad \text{..... IV.70}$$

For multicomponent systems, rigorous methods for the prediction of ψ_i, γ_i and f_i^{OL} are available as suggested by Prausnitz (113) while Dilfanian (115) provides an example of the application of these methods. However, for binary non-azeotropic systems at moderate pressures of up to 5 atm., if the vapour can reasonably be assumed to be a perfect gas, ψ_i can be taken as unity and, ignoring the Poynting correction, the vapour liquid equilibrium may be approximated by:

$$y_i P = \gamma_i x_i P_i^o(T) \quad \text{..... IV.71}$$

where P_i^o is the saturation vapour pressure of component i at the system temperature T.

The activity coefficients γ_i can be predicted using experimental data and either Van Laar, Wilson or NRTL equations. The choice largely depends on which equation best represents the vapour-liquid equilibrium of the system under consideration. The Van Laar equations have been used for the activity coefficient prediction in this research and these are

$$\log \gamma_1 = (2B-A)x_2^2 + 2(A-B)x_2^3 \quad \text{..... IV.72}$$

$$\log \gamma_2 = (2A-B)x_1^2 + 2(B-A)x_1^3 \quad \text{..... IV.73}$$

where

$$A = \frac{(x_1-x_2)\log \gamma_2}{x_1^2} + \frac{2 \log \gamma_1}{x_2} \quad \text{..... IV.74}$$

$$B = \frac{(x_2-x_1)\log \gamma_1}{x_2^2} + \frac{2 \log \gamma_2}{x_1} \quad \text{..... IV.75}$$

The constants A and B are normally averaged over at least four values calculated from experimental data at various temperatures to account for the variation of activity coefficient with temperature.

Saturation vapour pressure data are most conveniently related to temperature by the Antoine equation

$$\log P_i^o(T) = C_1 - \frac{C_2}{C_3+T} \quad \text{..... IV.76}$$

where the constants C_1, C_2 and C_3 can be evaluated from three sets of vapour-pressure-temperature data.

IV.4.6 PHYSICAL PROPERTY PREDICTION

Tray efficiency prediction by the A.I.Ch.E. method requires the knowledge of an almost complete spectrum of the physical properties of the liquid system ranging from the critical properties to the vapour and liquid diffusivities of the components. Usually, such data are not available and need to be estimated. The equations and the methods proposed for the estimation of the physical properties are given in Appendix B.

IV.5 SIMULATION OF BINARY DISTILLATION COLUMNS

The central theme in dynamic simulation is usually the solution of the differential equations that essentially constitute the mathematical model of the system being simulated. The philosophical approach to the solution of a single or a set of differential equations is an analogue of the principle of "causality" which states that the future can be predicted from a knowledge of the present. The connotation of this in mathematical sense is that if a variable, x obeys the deterministic differential equation

$$\frac{dx}{dt} = f(x,t)$$

the state (value) of x at time $t+\delta t$ depends only on the state of x at time t and not how x reached the state at time t. This principle is equally applicable to the solution of stochastic differential equations except that in this case it will be more relevant to talk about the probability law of x as opposed to its state. Therefore, if the state of a variable x at time t is known together with its differential equation, its state at time $t+\delta t$ can also be predicted.

If the dynamic simulator is being used to predict, say, a steady state starting from a given set of conditions, the closer the starting point to the steady state the less the effort needed to reach the steady state. As regards computer simulations, this effort is, simply, the computation time. Thus, a judicious choice

of the starting conditions can give us a head start in saving computer time. As far as binary distillation columns are concerned, life is somewhat easier in that a realistic set of starting conditions can easily be obtained by a steady-state shortcut method such as the McCabe-Thiele. This approximate steady-state can then be refined by the dynamic simulator more efficiently. The two versions of binary distillation column simulation compiled in this research adopt this technique to overcome the initialisation problem. The first simulator is based on Model I while the second one uses Model II. Both simulators offer a choice for tray efficiency calculation in case the experimental values of tray efficiencies are available.

The simulators can, therefore, be conveniently divided into two different parts namely,

(i) the initialisation by approximate steady-state calculations to obtain the temperature and composition profiles and the flow rates

(ii) the dynamic part to perform the dynamic simulation

IV.5.1 INITIALISATION

1. Specify a realistic separation; x_D and x_B.
2. Guess a reasonable value for the reflux ratio and fix x_D
3. Adjust the reflux ratio to achieve the specified separation by iterating around the reflux ratio until the calculated value of x_B is within a

tolerance of the specified value. This can be done by a Wegstein type algorithm to achieve speedy convergence (subroutine SDWEG). However, care must be taken to ensure that the computed reflux ratio is physically meaningful.

4. Perform a McCabe-Thiele steady-state calculation to obtain approximate temperature and composition profiles and vapour and liquid rates. If efficiency calculations are requested, compute approximate tray efficiencies based on these approximate profiles and flowrates (subroutine SSMODL).

The subprograms that perform these functions are named, SDWEG, SDSSWEG, and SSMODL respectively.

It must be noted that this exercise is purely for the initialization of the dynamic modules and its accuracy is of secondary importance. Thus if a reasonable set of temperature and composition profiles are available together with the corresponding vapour and liquid rates, then this exercise becomes redundant.

IV.5.2 ALGORITHMS

IV.5.2.1 THE MAIN PROGRAM

The algorithm for the main program segment is as follows:

1. Read in the physical data including:
   - (i) the separation for the steady-state calculations, total number of plates, number of components and the feed plate
   - (ii) the Brambilla equation constants
   - (iii) vapour-pressure-temperature data for the calculation of Antoine equation constants
   - (iv) temperature-composition data for the calculation of Van Laar equation constants
   - (v) the latent heats of vaporisation of the components
   - (vi) the specific heat capacity constants if model II is being used
   - (vii) if efficiency calculations are requested, then read in the physical properties of the components of the liquid system and the geometrical design information including tray type and dimensions
   - (viii) read in the integrator parameters and the print frequency
   - (ix) read in the frequency with which the efficiency calculations are to be repeated and the end of the simulation time
2. Compute reflux ratio for the specified separation

(subroutine SDWEG)

3. Compute approximate vapour and liquid rates and temperature and composition profiles and also efficiencies if requested (subroutine SSMODL).
4. Initialise the integrated variables in the dynamic simulator and adjust any number of the variables as necessary.
5. Set TIME=0, and zero all of the integrator pass numbers.
6. CALL the dynamic module.
7. If TIME is equal to ENDTIME, then stop.
8. Set TIME=TIME+DT; where DT is the integration step size.
9. Return to step 6 and continue.

IV.5.2.2 ALGORITHM FOR THE SOLUTION OF THE DYNAMIC MODEL I

In addition to the integrator parameters, certain flags are chosen to enable easy communication with the simulator in order to display the dynamic characteristics of selected trays during a run or to control the frequency of the efficiency calculations. These flags must be set before the dynamic simulator is entered.

The Algorithm

1. Store efficiency values if available and print information in accordance with the specified print interval.

2. Compute tray liquid hold-up and composition derivatives.
3. Integrate differential equations by calling the integrator : the SDINT subroutines.
4. Perform bubble point calculations in order to compute the equilibrium temperatures.
5. Compute the liquid rates leaving each tray from the truncated Brambilla equation.
6. Calculate the boil-up rate.
7. Compute efficiencies if requested and in accordance with the specified frequency.
8. Calculate the actual composition of the vapour leaving each tray.
9. Test for the step completion if the higher order integration methods are being used. If the step is not completed, return to step 2 and continue until the pass numbers of the higher integration methods are zeroed as signalled by the integrator.
10. Return.

IV.5.2_3 ALGORITHM FOR THE SOLUTION OF DYNAMIC MODEL II

This algorithm is much the same as the algorithm for the solution of model I except that the step 6 is excluded and the following calculations are performed instead:

(i) compute enthalpies of the liquid and vapour streams leaving each stage

(ii) calculate the enthalpies of the feed and reflux

streams

(iii) compute the individual vapour rates leaving each stage starting from the reboiler

The complete listings of the programs are given in Appendix B.1.1 (Microfishe)

IV.6 STIFFNESS ASPECTS OF DISTILLATION COLUMN SIMULATION

In a system simulation stiffness essentially materializes when the system's differential equations have very small time constants compared with the dominant time constants of the system. Thus if the integration step size used to solve them is not sufficiently small, the simulation can become very inaccurate, if not unstable or divergent.

Stiffness problem in distillation simulation are even more chronic in that none of the compositions can exceed unity. Once a composition exceeds unity due to the inaccuracies induced by a large integration step size, then the bubble point calculations will almost certainly diverge. In such cases, there exists a critical step size that would accommodate any stiffness situation and beyond which the integration step size must not be increased. Various attempts have been made to relate the critical step size to the largest eigenvalue of a linear system (117). This approach is by no means a panacea inasmuch as it only covers linear systems and, moreover, it is dependent upon the integration method.

In a complex non-linear system such as distillation, the critical step size must eventually be determined by trial-and-error and a few computer runs. Naturally, a small critical step size means very long running times and this may not be desirable. Thus attempts must be made to compensate for the consequen-

tial loss of computational efficiency by other means. Under these conditions, the following techniques were implemented and found to be effective:

(i) the number of interstep bubble point iterations were reduced considerably by using the temperature of the previous integration step as the guess temperature for the present step

(ii) the tray efficiency need not be calculated at every step but at a predetermined frequency as they are almost time-invariant during a run

(iii) the use of a variable step integrator

C H A P T E R F I V E

OPEN-LOOP SIMULATION RESULTS and EXPERIMENTAL VERIFICATIONS

V.1 OPEN-LOOP SIMULATION STUDIES

The simulators discussed in the previous chapter were used to simulate the 3-inch, 10 sieve-tray distillation column that was discussed in Chapter III. In order to enable comparison between the predictions of the two simulators, it was assumed that the feed and reflux streams entered the column as saturated liquids at their bubble points. The critical step size for this column was found to be 0.4×10^{-4} hour and since these were purely theoretical studies intended to achieve an understanding of the dynamic character of the column, it was decided to adhere to the simple Euler integration method to avoid excessive running times. It was also assumed that the column was under open-loop conditions and aside from the flow and heat input regulations, the only control actions were due to the reflux drum and reboiler level controllers. These conditions are sometimes referred to as the "natural control" conditions. The schematic diagram of the column under natural control conditions is depicted in Figure V.1. The binary liquid system was trichloroethylene and tetrachloroethylene with the trichloroethylene being the most volatile component with a feed mole fraction of 0.4. The geometric configuration of the column is discussed in Chapter III while the properties of the liquid system are given in Appendix C.

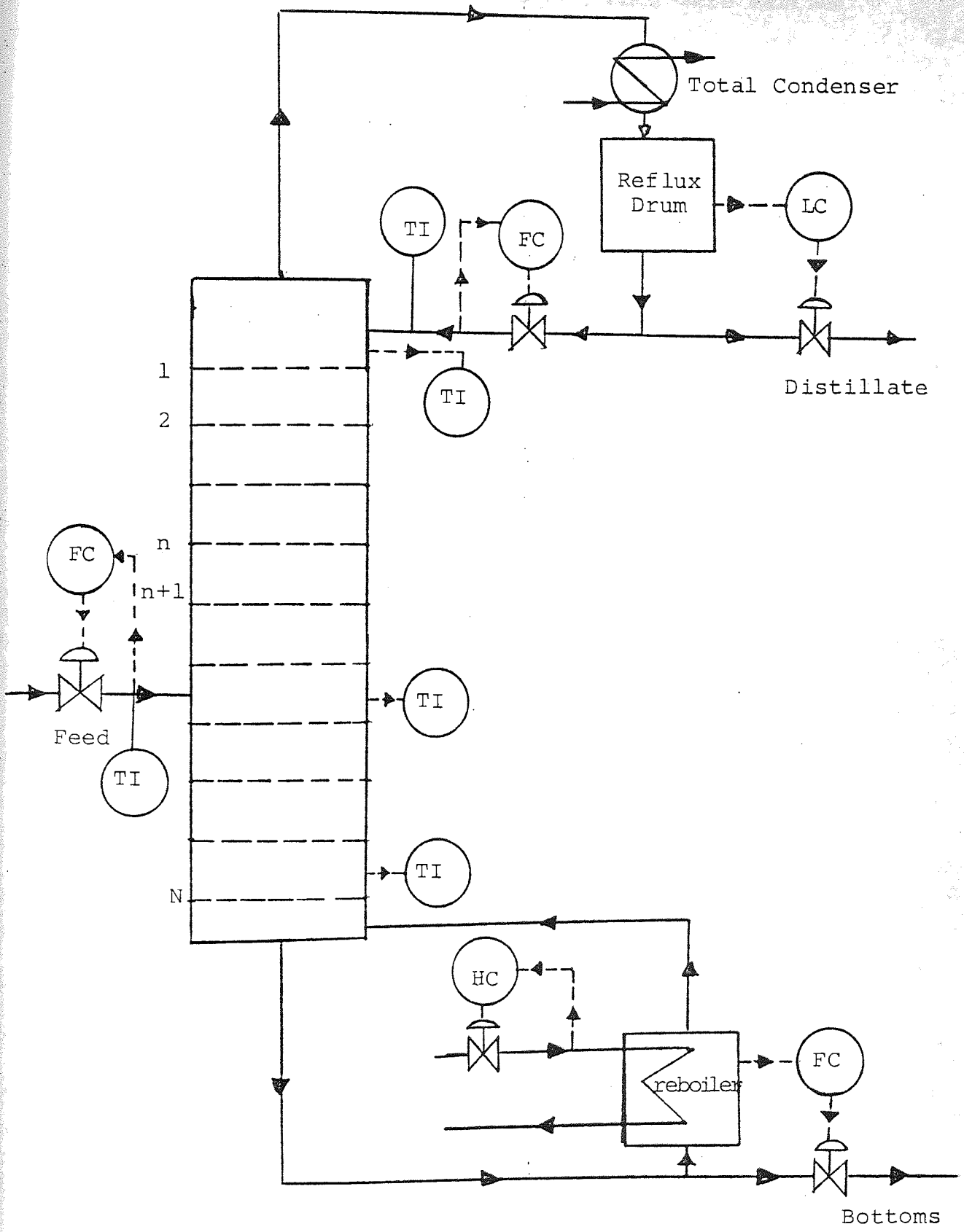


FIGURE V.1 The Schematic Diagram of the Column under "Natural Control"

The following computer experiments were carried out:

(i) the prediction of a more accurate steady state starting from the approximate McCabe-Thiele predictions: Figures V.2 and V.3

(ii) the response to a step change in the feed rate introduced at steady state: Figures V.4 and V.5

(iii) the response to a step change in the feed composition introduced at steady state: Figures V.6 and V.7

Since the effects of subcooling of the feed and reflux streams on the column's performance were unknown, it was decided to use the simulator based on model II, discussed in Chapter IV, to study these effects. This was another example of how dynamic simulation could be effectively used to obtain a deeper insight into the behaviour of different processes. In this context, one more simulation experiment was carried out to study the response of the column to the step changes in the feed and reflux temperatures. The results are shown in Figures V.8 and V.9.

During these experiments the feed rate was chosen as 10 mole/hr. and the reboiler holdup was 60 moles. These simulation studies were necessary to

(i) ensure that the simulators were functioning properly

(ii) achieve an understanding of the dynamic character of the column

Figure V.2
Simulation Experiment No.1
Steady-State Prediction by the Two Models starting from the McCabe-Thiele Approximation

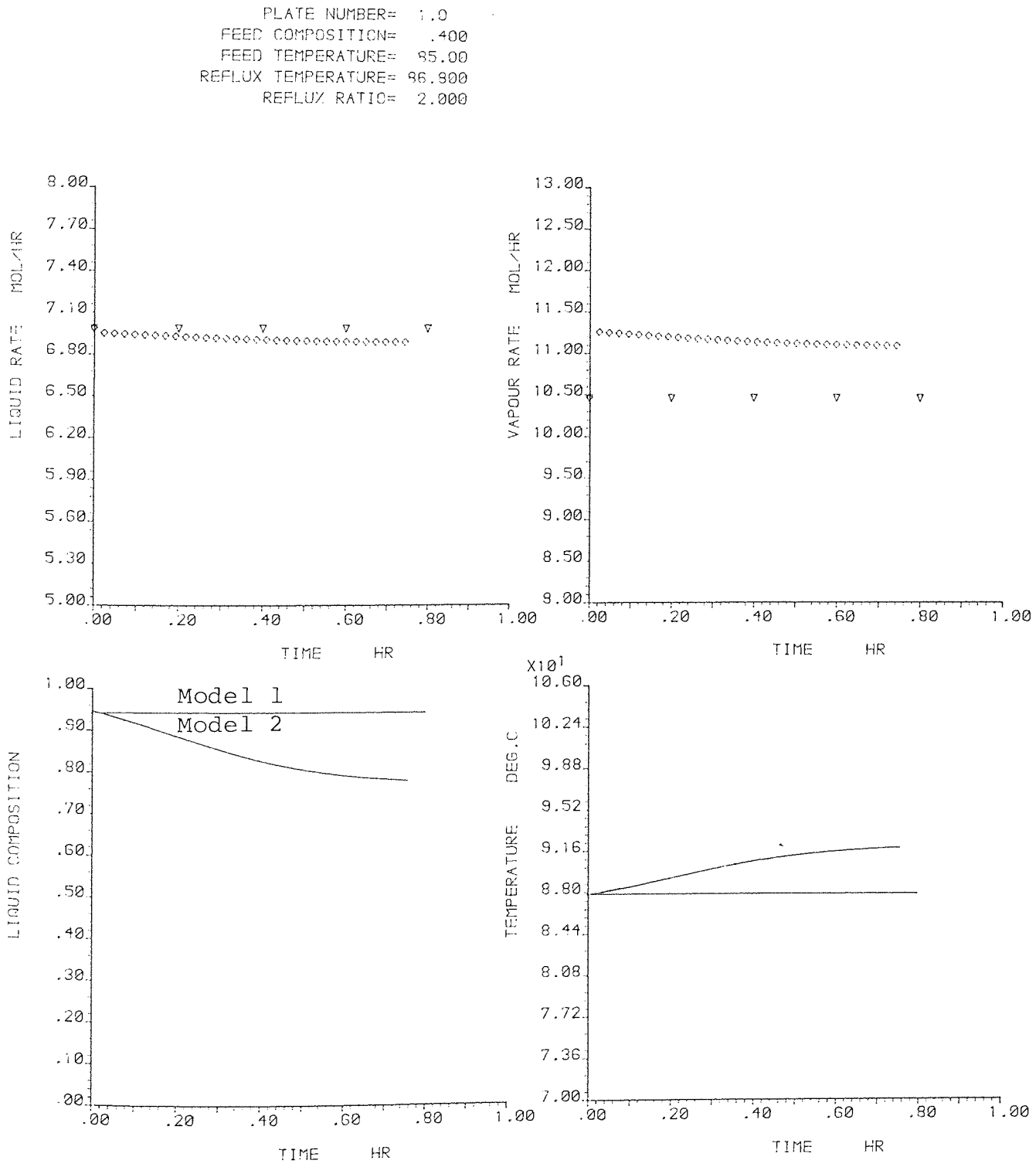


Figure V.3
Simulation Experiment No.1 continued

PLATE NUMBER= 20.0
FEED COMPOSITION= .400
FEED TEMPERATURE= 85.00
REFLUX TEMPERATURE= 86.900
REFLUX RATIO= 2.000

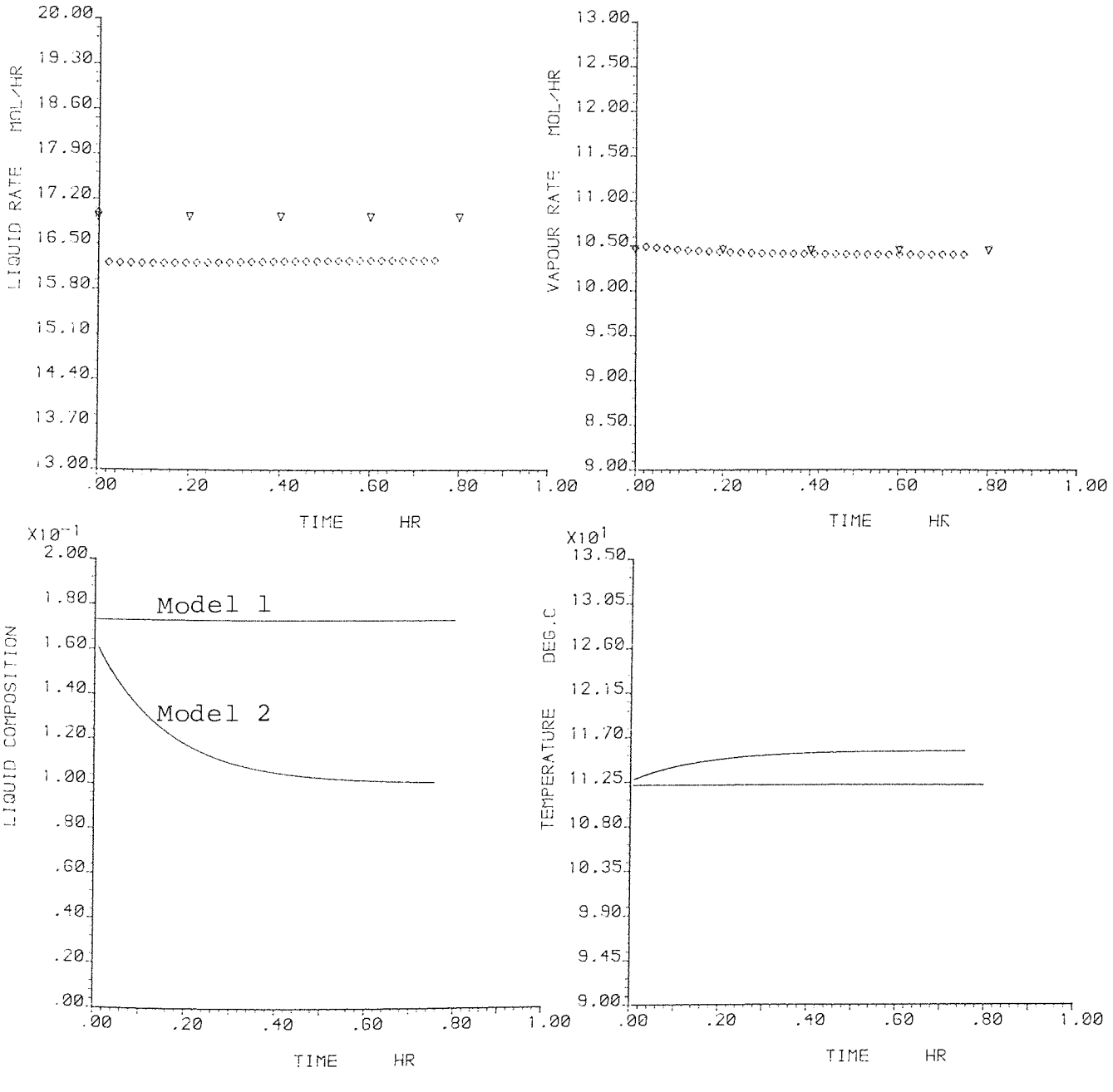


Figure V.4
Simulation Experiment No.2
The Open-Loop Response of the Column 10% Step Increase in the Feed Rate

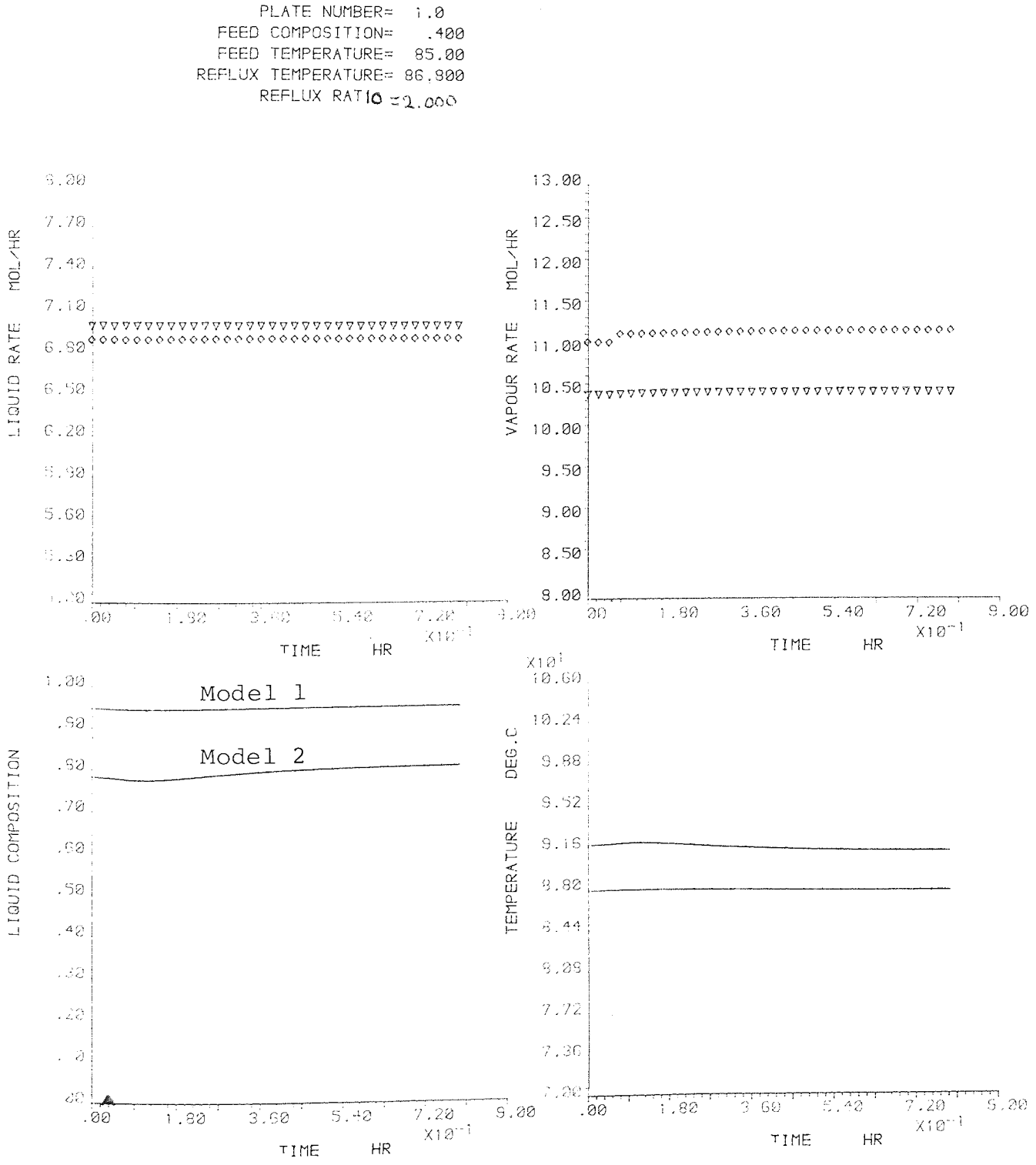


Figure V.5
SImulation Experiment No.2 continued

PLATE NUMBER= 10.0
FEED COMPOSITION= .400
FEED TEMPERATURE= 85.00
REFLUX TEMPERATURE= 86.900
REFLUX RATIO= 2.000

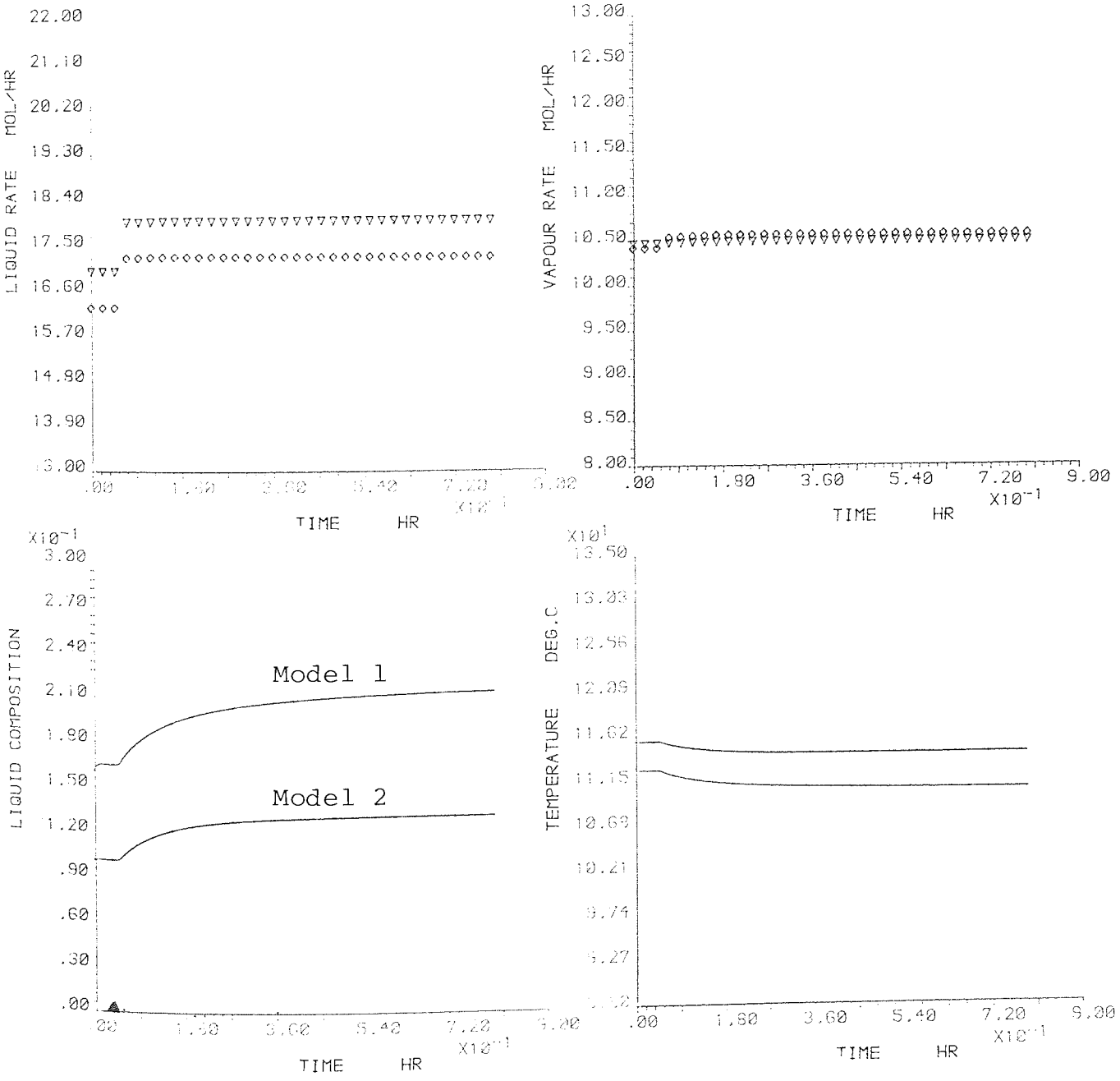


Figure V.6
Simulation Experiment No.3
The Open-Loop Response of the Column to 10% Step Increase in the Feed Composition

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FEED COMPOSITION= .400
FEED TEMPERATURE= 85.00
REFLUX TEMPERATURE= 86.900
REFLUX RATIO= 2.

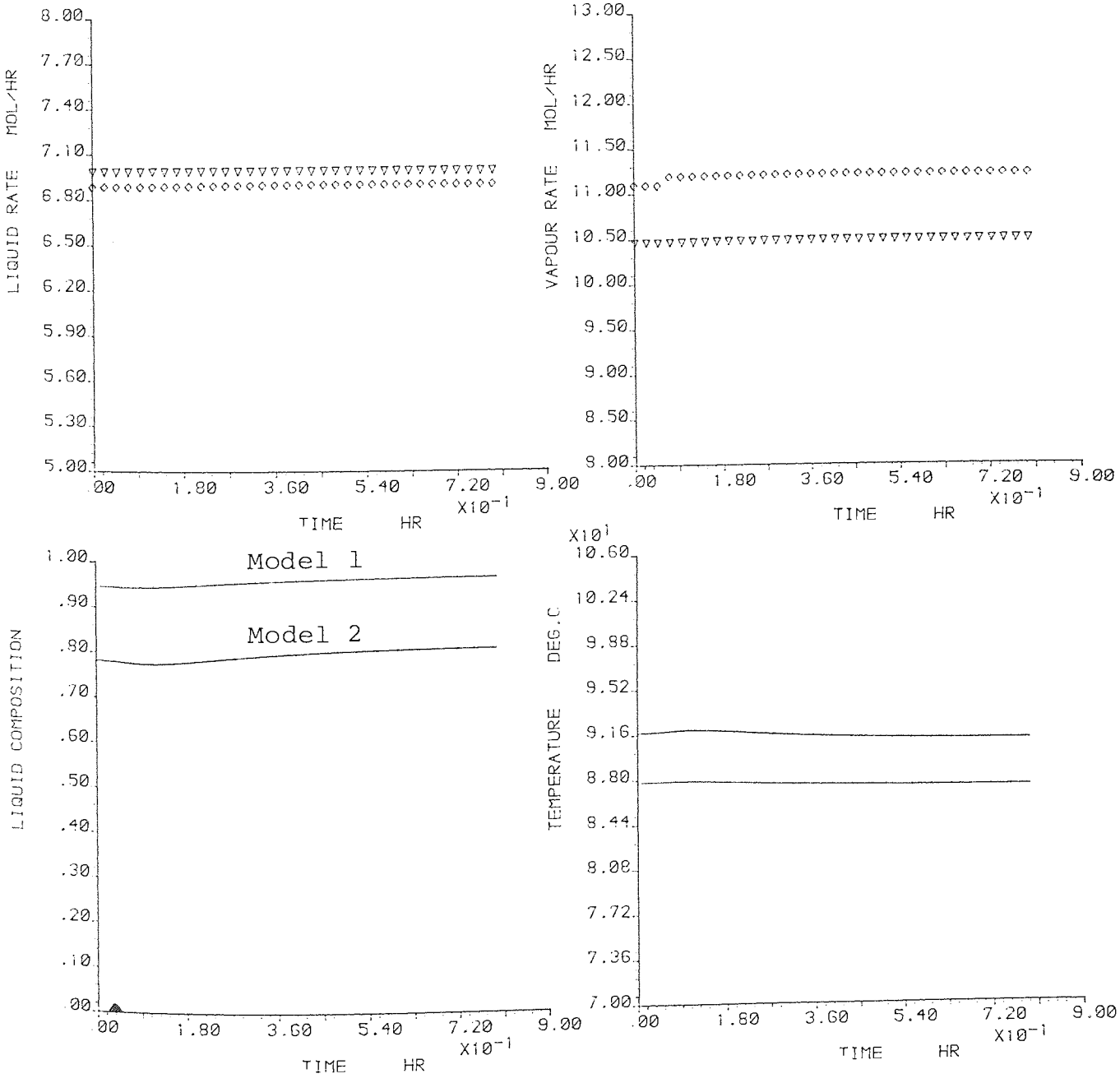
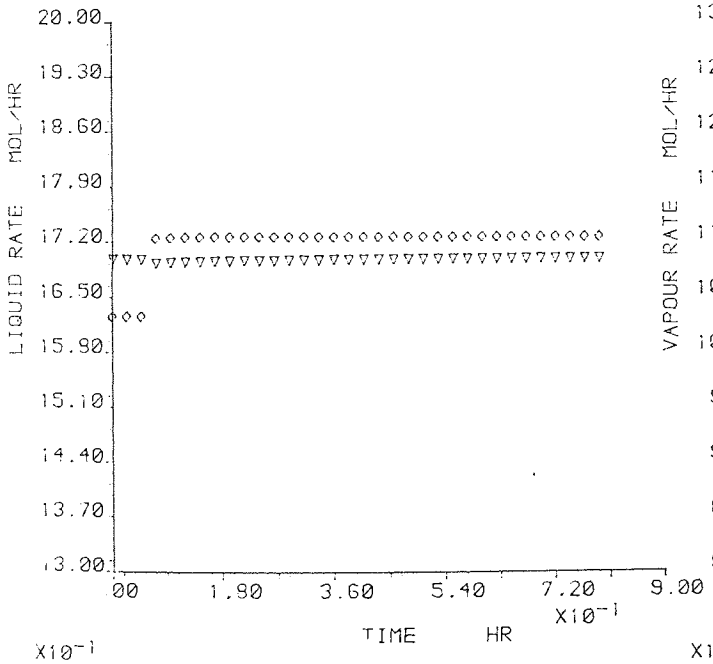
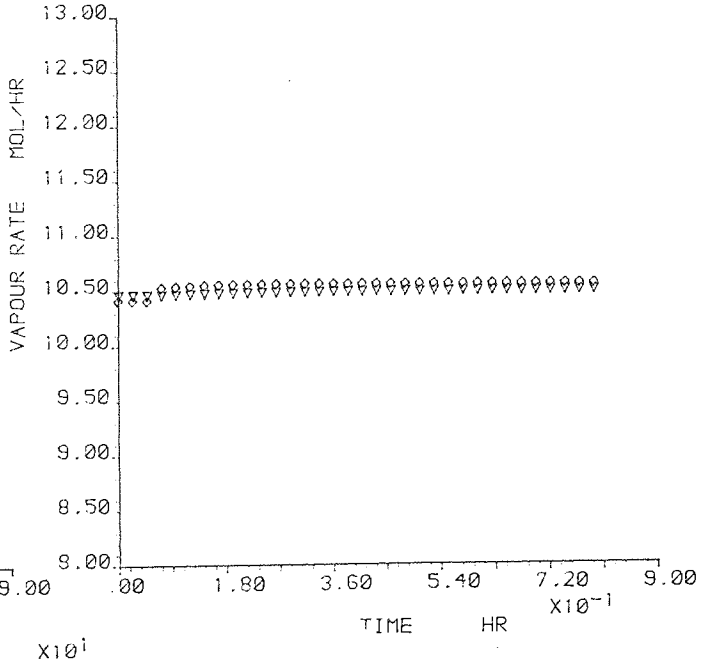
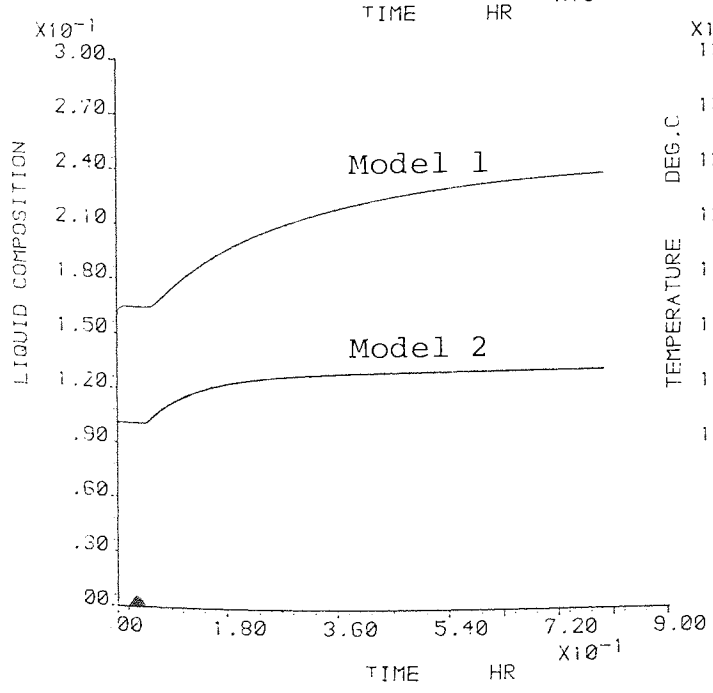


Figure V.7
Simulation Experiment No.3 continued

PLATE NUMBER= 10.0
FEED COMPOSITION= .400
FEED TEMPERATURE= 85.00
REFLUX TEMPERATURE= 86.900
REFLUX RATIO= 2.000







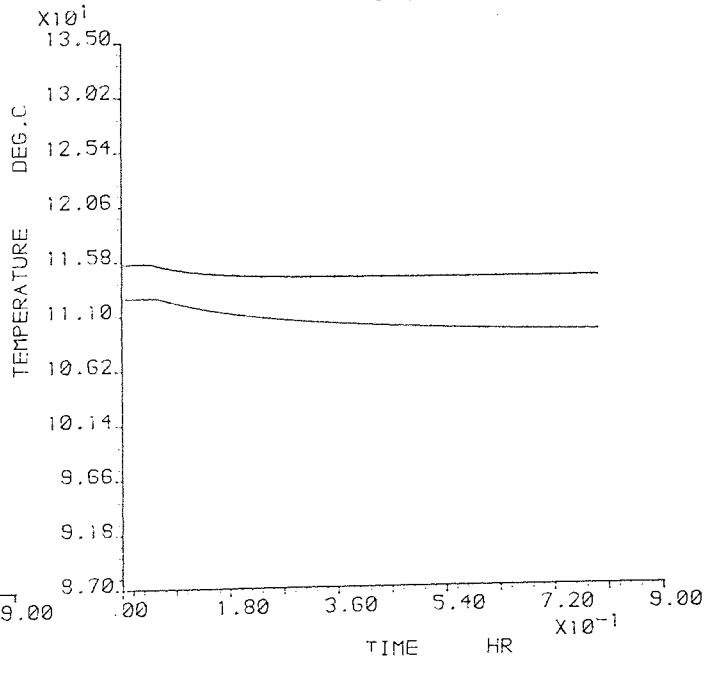


Figure V.8
Simulation Experiment No.4
The Open-Loop Response of the Column to Consecutive Step Decreases in the Feed and Reflux Stream Temperatures down to the Room Temperature Predicted by the Simulator No.2

PLATE NUMBER= 1.0
FEED COMPOSITION= .400
FEED TEMPERATURE= 85.00
REFLUX TEMPERATURE= 86.900
REFLUX RATIO= 2.000

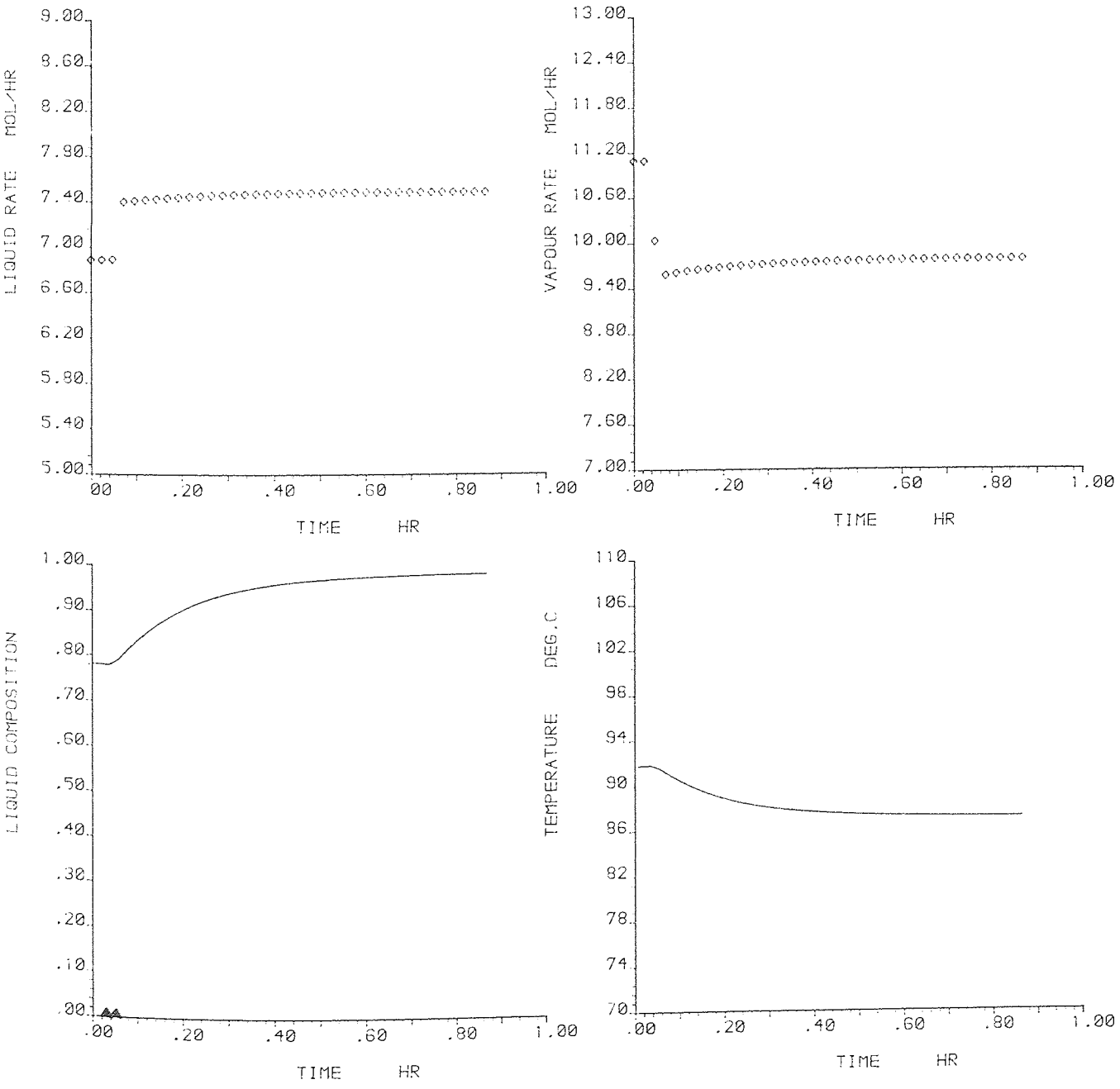
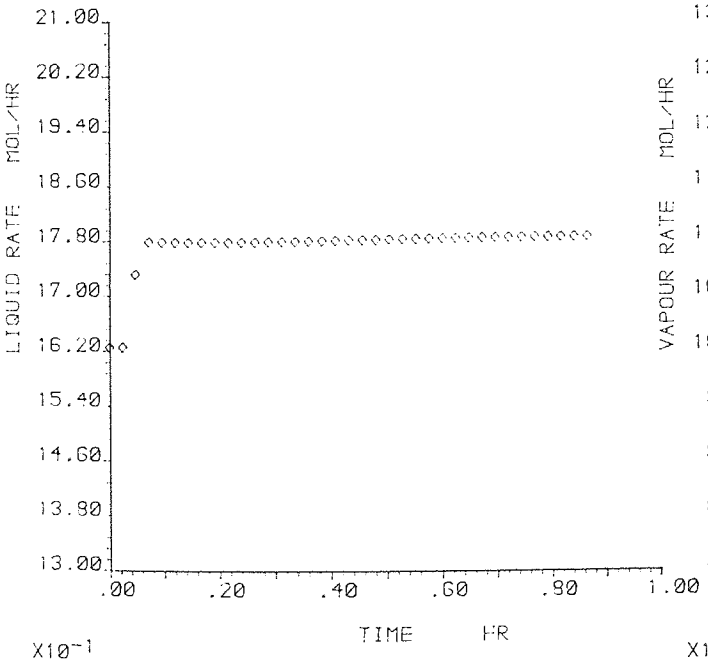
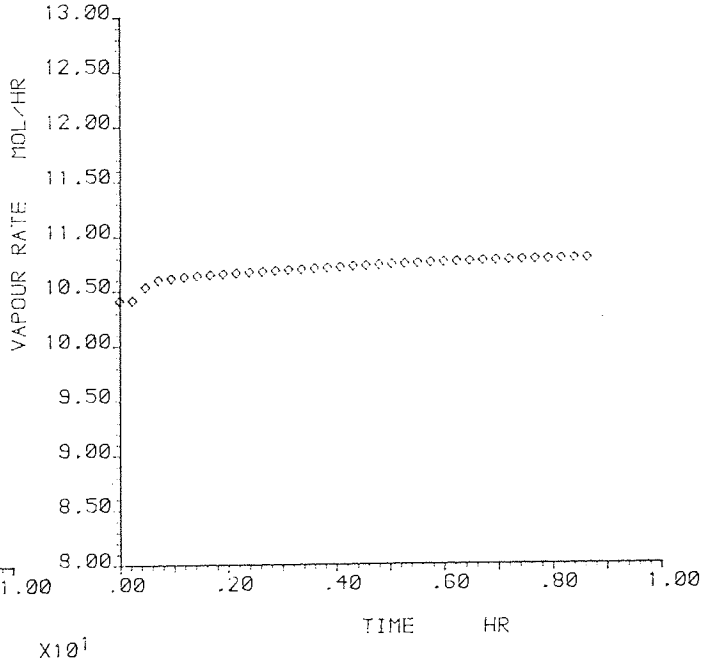
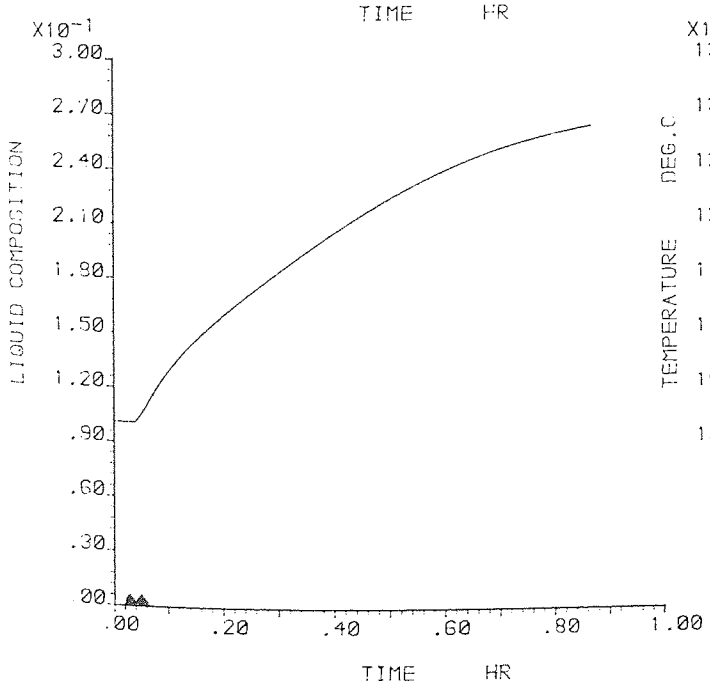


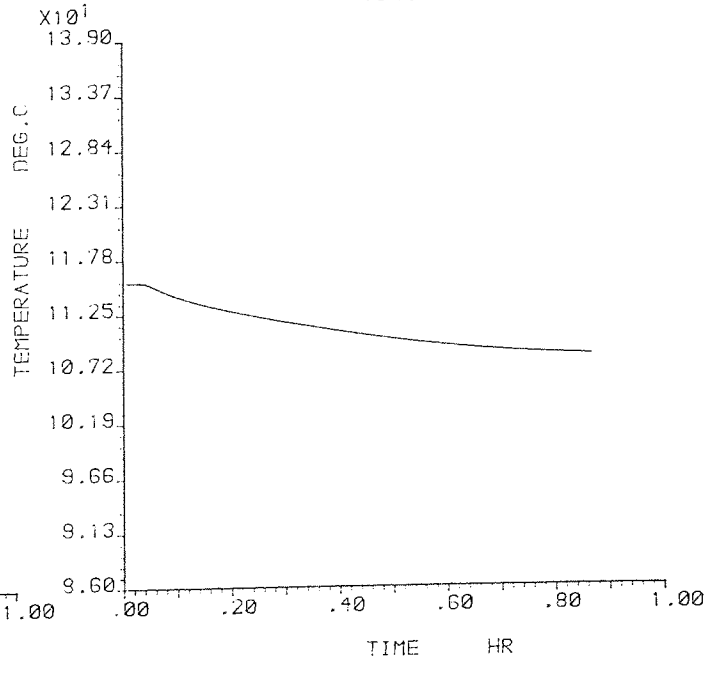
Figure V.9
Simulation Experiment No.4 continued

PLATE NUMBER= 10.0
FEED COMPOSITION= .400
FEED TEMPERATURE= 85.00
REFLUX TEMPERATURE= 86.000
REFLUX RATIO= 2.000









(iii) modify the instrumentation necessary for the dynamic studies and control of the actual column. E.g. as a result of the simulation experiment No.4, it was decided to measure the feed and reflux stream temperatures

(iv) compare the performances of the two models for binary distillation discussed in Chapter IV. We shall return to this point during the design of the Kalman filters

The simulations were run on the University's 1904S computer. Exact statistics for the running times are difficult to provide as it is virtually impossible to estimate the overheads. Also, the frequency with which the efficiency calculations are repeated has a strong bearing on the running times. Nonetheless, despite these variables it can be assumed that the ratio of the simulation time to real computer time is approximately 4 to 1 when the efficiencies are recomputed every 3 minutes and the results are also printed out every 3 minutes.

V.2 THE OPEN-LOOP EXPERIMENTS

In order to ensure that simulator II, discussed in Chapter IV, is a reasonable representation of the static and dynamic characters of the column, it was decided to check its predictions of the topmost and lowermost tray temperatures experimentally. Thus, the following open-loop experiments were carried out during which the column operated under "natural" control only (see Figure V.1). These were:

(i) steady-state operation

(ii) the response to a step change in the feed rate

The process equipment is depicted in Figure III.1, in Chapter III. The two proportional level-controllers used to control the reflux drum and the reboiler levels were tuned on-line such that steady levels were maintained by the manipulations of the top and bottom product valves: as shown in Figure V.1. The feed, reflux and heat input rates were maintained by refreshing the settings of their associated analogue output channels.

The liquid system components were trichloroethylene and tetrachloroethylene whose properties are tabulated in Appendix C.

A software package known as the HADIOS Executive is available which enables the user to communicate with the column, through HADIOS, from a BASIC program. This package is intended to enable the user to access

the column regularly at a chosen time frequency. The version of this software used by Webb (27) has been modified in this research. These modifications are hoped to render the package more flexible in the following ways:

(i) they provide a simpler communication scheme with the package

(ii) they enable the user to service more than one digital output channel at a time

(iii) they enable the electrical noise to be smoothed out to some extent during the scanning of the analogue input channels

The listings of the latest version of the HADIOS Executive and its modifications for this research are given in APpendix D.

V.2.1 THE STEADY-STATE EXPERIMENTS

A number of steady-state experiments were carried out on the distillation column under the same operational conditions. The steady-state temperature measurements were checked against the predictions of the simulator II. The procedure followed is:

1. Carry out the experiment ensuring that the column runs at steady-state for at least 20 minutes and record the following information for about 20-30 minutes.
   (i) the top and bottom tray temperatures
   (ii) the feed rate, composition and temperature
   (iii) the reflux rate and temperature
   (iv) the heat input rate
   (v) the reboiler and reflux drum levels
2. Feed all the information obtained in step 1 (except the tray temperatures) into the simulator and drive the simulator to steady state.
3. Plot the tray responses on the 1904S computer with the experimental tray temperatures, from step 1, superimposed on their predicted counterparts.

Since the simulator assumes adiabatic operational conditions, the actual heat input rate recorded during the experimental runs must be corrected for the inherent heat losses that take place during the operation of the column. In other words

$$Q_{adiabatic} = Q_{actual} - \delta Q_{lost}$$

A typical set of the experimental input data used to test the simulator is given in Table V.1. since the standard print-out of the simulator is based on a feed rate of 10 moles/hr., all the rates and holdups need to be scaled. The simulator expects the scale factor to handle the calculations such that the actual experimental conditions are simulated.

The details of the calculation procedure for the estimation of the heat losses are given in Appendix C. The graphic results are shown in Figures V.10 and V.11. The accuracy of the steady-state temperature predictions were found to be within $\pm 0.6^{o}C$. for the topmost and lowermost trays.

V.2.2 THE RESPONSE TO A STEP INCREASE IN THE FEED RATE

Amongst the possible load changes that can be introduced, throughput changes are normally more testing as far as the response and operation of the column is concerned. It was therefore decided to adhere to this type of disturbance because if the prediction of the column's response to throughput changes is reasonably accurate, it could be assumed that the prediction of its response to composition changes could also be made with a comparable accuracy. Moreover, to ensure that the simulator is a reasonable representation of the column under extremely transient conditions, it was decided to introduce a rather unrealistically large step increase of about 40 per cent in the feed rate. In real life, most columns usually operate within 10 to 15 per cent of their full capacities and, therefore, step changes of more than 10 per cent are not expected or, if expected, they are usually buffered by a storage tank that precedes the column. However, it was thought to be necessary to test the simulator under extreme conditions to ensure its robustness. The experimental and simulation procedures were much the same as the steady-state case except that having run the column at steady state for 15 minutes, the feed rate is increased and an estimate of the time taken for the disturbance to reach the column is also made. This is important in

that this time lag must be allowed for in the simulation of the upset.

A typical set of the dynamic experimental results have been superimposed on their corresponding theoretical predictions and shown in Figures V.12 and V.13. The experimental details are given in Table V.1.

It was found necessary to use the Manchester Regional Computer for the simulation of the experiments since it was decided that the fourth-order Runge-Kutta integration method should be used to enhance the computational accuracy. The accuracy of the simulation predictions under transient conditions were also found to be in the order of $\pm 0.6^{\circ}C$ as regards the topmost and lowermost tray temperatures.

Figure V.10
Comparison of the Experimental and Predicted Steady-State Tray Temperatures

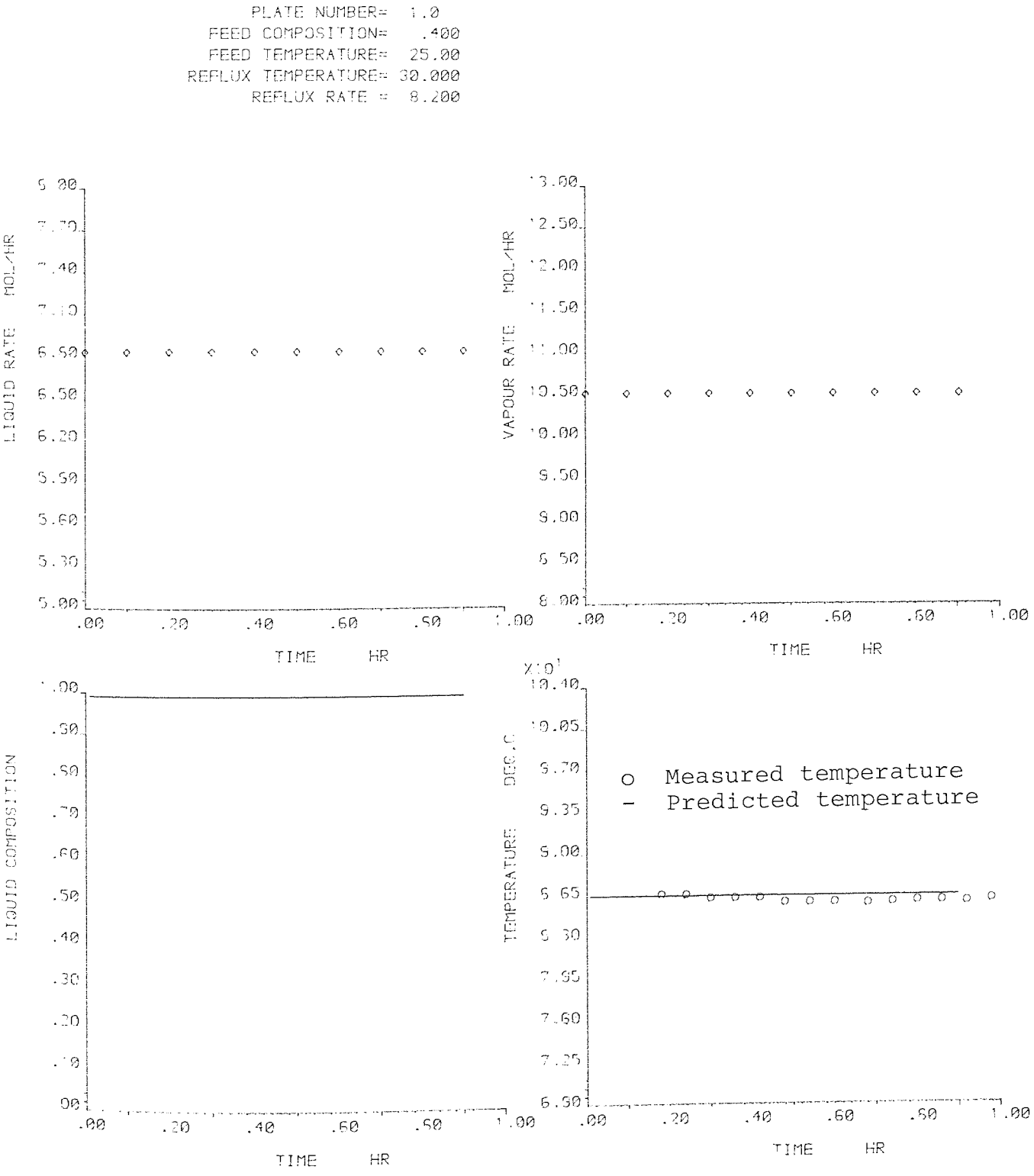


Figure V.11
Steady-State Comparison Continued

PLATE NUMBER= 10.0
FEED COMPOSITION= .400
FEED TEMPERATURE= 25.00
REFLUX TEMPERATURE= 30.000
REFLUX RATE = 8.200

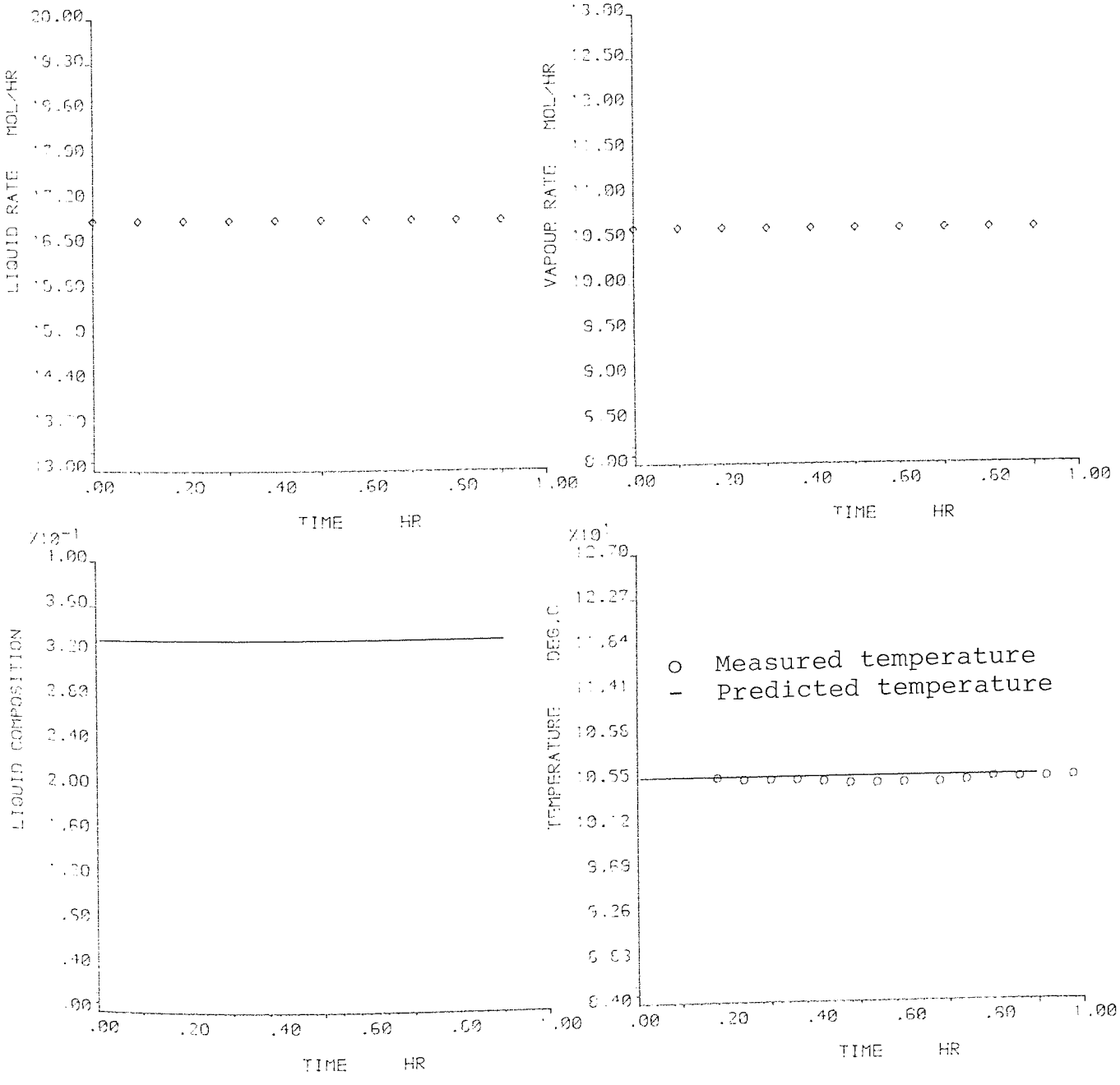


Figure V.12
Comparison of the Experimental and Predicted Open-Loop Tray Temperature Responsesto 42% Step Increase in the Feed Rate

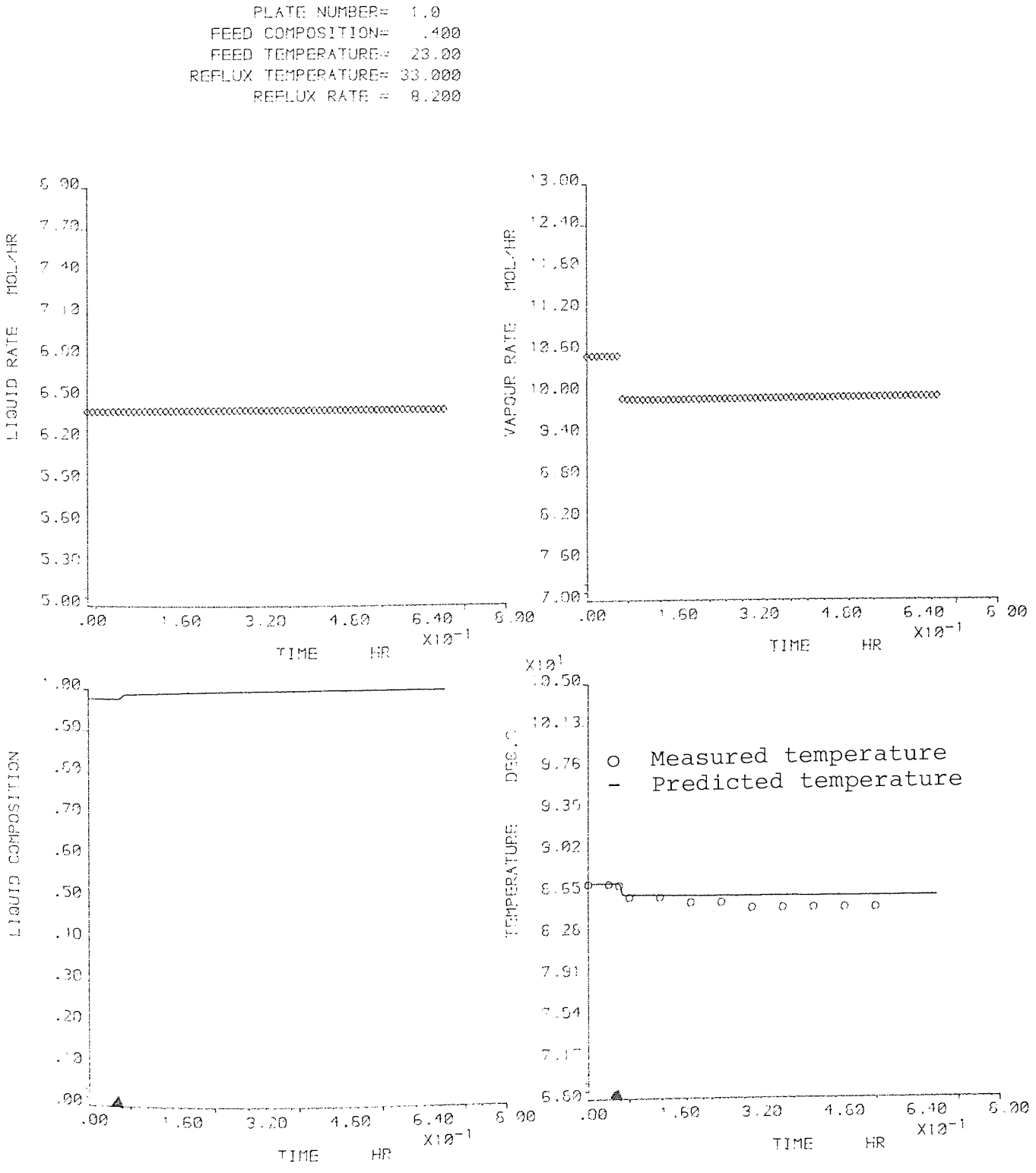
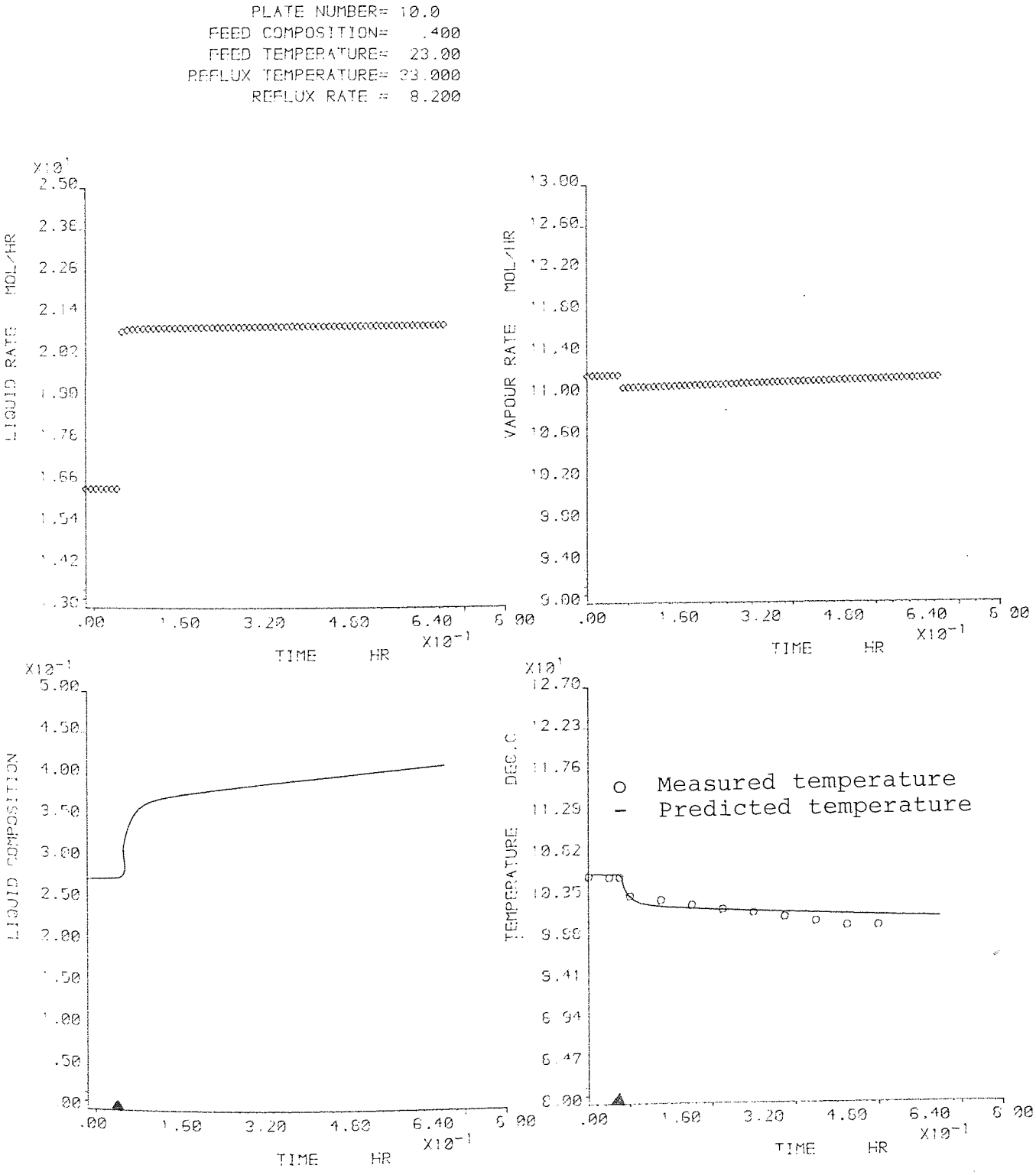


Figure V.13
Open-Loop Experimental and Predicted Responses of the Column to a 42% Step Increase in the Feed Rate Continued



Steady State Experimental Details		
Feed rate	= 100	mole/hr.
Reflux rate	= 82	mole/hr.
Reboiler Holdup	= 100	moles
Reflux Drum Level	= 60	moles
Feed Composition	= 0.40	
Feed Temperature	= 25	^{o}C
Reflux Temperature	= 30	^{o}C
Actual Heat Input	= 4805	kJ./hr.
Estimated Heat Losses	= 1195	kJ./hr.
Scanning Interval	= 2.0	sec.
Unsteady State Experimental Details		
Feed Rate	= 100	moles/hr.
Reflux Rate	= 82	moles/hr.
Reboiler Holdup	= 100	moles
Reflux Drum Holdup	= 60	moles
Feed Composition	= 0.4	
Feed Temperature	= 27	^{o}C
Reflux Temperature	= 33	^{o}C
Actual Heat Input	= 4805	kJ./hr.
Estimated Heat Losses	= 1195	kJ./hr.
Size of the Step Change	= 0.42	
Scanning Interval	= 2.0	sec.

Table V.1 - The Experimental Details of the Steady-State Experiment No.5 and the Unsteady State Experiment No.7, are tabulated

C H A P T E R S I X

THE DESIGN OF ESTIMATORS AND THEORETICAL DEVELOPMENTS

VI.1 THE NEED FOR STOCHASTIC MODELS AND ESTIMATION IN RELATION TO CONTROL

There are several reasons for the use of stochastic models and estimation as an aid to control in the Chemical Process systems.

(i) the limitations of deterministic models

(ii) unknown system inputs

(iii) imprecise measurements and the lack of availability and infrequency of primary control measurements

These points will now be discussed briefly.

1. The Limitations of Deterministic Models

Given a physical system which is to be controlled, an engineer attempts to develop a mathematical model of the system that adequately represents some aspects of the behaviour of that system. This is usually done by delineating the variables describing the process and then connecting them via certain causal relationships or physical laws. At this stage, such factors as physical insights, empirical testing can be instrumental in establishing the inter-relationships among certain variables of interest, inputs to the system and outputs from the system.

With such a mathematical model and the tools provided by system and control theories, it is then possible to investigate the system structure and modes of response and design controllers that provide

appropriate inputs to generate system responses - i.e. a control strategy.

On the implementation of this strategy on the real system, it is very likely that the system will not behave as expected due to inaccuracies in the mathematical model. Here, one might choose to sophisticate the model further and further in return for more accurate representations. There will, however, come a time when nothing more can be gained by further deterministic sophistications. This level of sophistication is normally identified as the "noise level". It can be confidently asserted that even at levels approaching the noise level, no deterministic mathematical model is perfect. If the mathematical model of the system is not as good as it can be, then the control strategy cannot as effective as it can be.

This provides the first incentive for resorting to stochastic models.

2. Unknown System Inputs

For the sake of argument, let us suppose that it is possible to achieve a perfect system model deterministically and the engineer then proceeds to design a controller based on this model. Almost invariably, the controller synthesis will then be based on preselected deterministic inputs. In actuality, real systems are not only driven by our own control inputs, but also by disturbances which we can neither control nor model deterministically. Thus, in the unlikely

event of achieving such a perfect deterministic model, the devised control strategy may still not be good enough.

3. Imprecise Measurements

Implicit in the control of any system is the need for some information about the system. This information can only be achieved by measuring some of the variables of the system. The variables that can be measured may suffer from the following disadvantages:

(i) they may be corrupted as sensors do not provide perfect and complete data

(ii) they may not be what we want to measure

Generally, sensors do not provide all the information that we would like to know : either a device cannot be devised to generate a measurement of a desired variable or the cost of including such a measurement is prohibitive. In other situations, a number of different devices yield functionally related data, and one must then ask how to generate a best estimate of the variables of interest based on partially redundant data. Not only do the sensors not provide exact readings, but also they introduce their own system dynamics and distortions. Furthermore, these devices are almost invariably noise corrupted. Imprecise measurement means imprecise control and one way to refine noisy measurements is by stochastic estimation.

A good example of how control is complicated by the problems associated with the on-line measurement of a tray composition occurs in distillation. On-line analysers are expensive and/or include such large time lags that makes it difficult to design even a reasonably effective feedback control system. Here an estimator can be used to estimate the tray composition from a secondary measurement such as tray temperature which is easy to measure. Control can then be based on this estimated composition.

VI.2 THE KALMAN FILTER

The concept of Kalman filtering has already been introduced briefly in section II.4.1. The method of implementation of filtering philosophy in on-line and off-line applications is depicted in Figure VI.1.

A Kalman filter is simply an optimal recursive data processing algorithm. There are many ways of defining optimal, dependent upon the criteria chosen to evaluate performance. It can be shown (137), that under the assumptions made in the formulation of the Kalman filter, the filter is optimal with respect to virtually any criterion that makes sense. One aspect of this optimality is that the Kalman filter incorporates all information that can be provided to it. It processes all available measurements, regardless of their precision, to estimate the current values of the variables of interest with the use of

(i) knowledge of the system and measurement dynamics (filter model(s))

(ii) the statistical description of the system noises, measurement errors, and the uncertainty in the dynamics models (R and Q matrices)

(iii) any available information about initial conditions of the variables of interest ($\bar{x}(t_o)$ and $P(o,o)$)

The word "recursive" means that the Kalman filter does not require all previous data to be kept in

storage and reprocessed every time a new measurement is taken. This is of vital importance to the practicality of filter implementation on digital computers.

The basic assumptions made in the Kalman filter formulation are:

(i) a linear system model

(ii) whiteness of the noise

(iii) Gaussian distribution of the noise

The use of a linear model is not restrictive. If non-linearities do exist, the typical engineering approach is to linearize about some nominal point or trajectory to achieve a perturbation or error model (see the extended Kalman filter). There are also means of developing non-linear filters (16).

"Whiteness" implies that the noise value is not correlated in time. As a result the knowledge of the value of the noise now in no way helps in predicting its value at any other time. In other words, all the values of the noise are "mutually independent".

Whereas Whiteness pertains to time or frequency relationship of noise, "Gaussianness" is related to its amplitude. Thus, at any single point in time, the probability density of a Gaussian noise amplitude takes on the shape of a normal bell-shaped curve. This assumption can be justified physically by the fact that a system measurement noise is typically caused by a number of small sources. It can be shown mathematically that when a number of independent

random variables are added together, the summed effect can be described very closely by a Gaussian probability density, regardless of the shape of the individual densities.

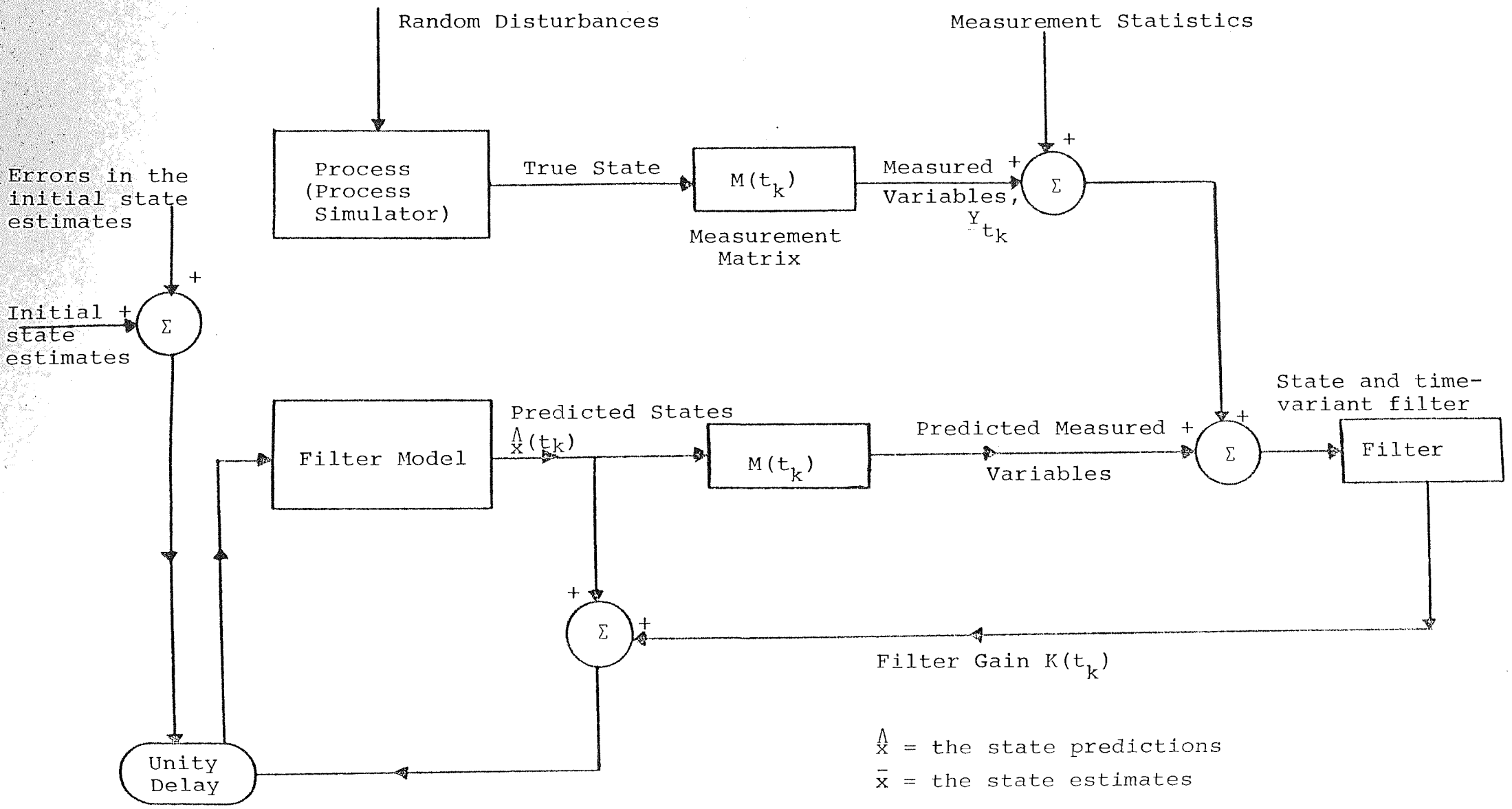
The practical justifications for using a "White Gaussian" noise in stochastic models are:

(i) it makes the mathematics more tractable

(ii) it is completely defined by its first and second order statistics

Therefore, in describing a dynamical system stochastically, almost invariably, it pays to adhere to the White Gaussian noise processes.

FIGURE VI.1 - Estimation Procedure in On-line and Off-line Applications



$$\bar{x}(t_k) = \hat{x}(t_k) + K(t_k)\,(Y(t_k) - M(t_k)\hat{x}(t_k))$$

V1.3 THE DESIGN OF KALMAN FILTERS

Despite the mathematical formalism of the Kalman filter approach, a substantial amount of engineering insight and experience is required to develop an effective operational filter. Mathematical models of both the system structure (state dynamics and output relations) and uncertainties are inherently embodied in the Kalman filter structure. However, obtaining an "adequate mathematical model upon which to base the filter" is the crux of the design problem. Even once a particular model is chosen as appropriate for a given application, a considerable effort may still be needed to obtain appropriate numerical evaluation of the coefficients within the model - especially the covariance matrices. This process will henceforth be referred to as "filter tuning". It essentially involves an iterative search for the coefficient values that yeild the optimum estimation performance from a particular filter structure.

Moreover, the design must meet the constraints of the on-line computer time, memory and wordlength available. These considerations dictate a philosophy of using as simple a filter as possible that yields adequate results. Consequently, it might be that one is forced to exploit basic modelling alternatives to achieve a simple but adequate filter. Modelling complexities might have to be added or deleted as the performance needs and practical constraints require.

Evaluation of true performance capabilities of any filter is of critical importance in the design procedure. Although a Kalman filter computes an error covariance internally, this is a valid depiction of the true errors committed by the filter only to the extent that the filter's own system model adequately portrays the true system behaviour. It is possible for the filter not to perform as well as it "thinks" it does. If the computed error covariance matrix is inappropriately small, the computed gain will also be small. This means that the filter weights its internal system model too heavily and disregards the data from the "real world" unduly. This phenomenon will lead to filter estimates not corresponding to the true system performance with a simultaneous indication by the filter through its computed covariance that all is well. Usually, under these circumstances the filter exhibits some peculiar behaviour. For instance, if the inaccuracies of the filter's system model are not properly allowed for, the estimates may diverge gradually or the filter may fail to track the estimated parameters if any.

It is generally felt that evaluation of the true performance of any Kalman filter is best accomplished by simulation. This is the reason why simulation is regarded as being an important preliminary to the design of Kalman filters.

VI.4 OBSERVABILITY

Observability is a property of a specific state space representation for a system, rather than of the system itself. Thus certain state space models will be more suitable for estimation than others, even though both might portray the input-output characteristics of the system.

The concept of observability in linear systems is well established and the methods available for assessing observability are generally applicable (137). However, in non-linear systems, although this concept has been considered by many workers, some of whom have tried to quantify observability, there are, as yet, no general methods of assessing observability. Experience has, however, shown that this is one issue which has to be settled at the simulation stage of designing a Kalman filter and one obvious way to combat unobservability is to increase the number of measured variables. Experience has also shown that the system becomes unobservable when some of the estimates oscillate about the true states and the related diagonal elements in the computed error covariance matrix, $P_{n,n}$, become unduly large - larger than the corresponding state variables themselves in some cases. For example, if a state variable happens to be a mole fraction which can only have a maximum value of 1 and its computed variance is 2, then its estimate will be somewhat meaningless.

VI.5 THE COVARIANCE MATRICES : Q AND R

The error covariance matrices Q and R are not computed by the filter algorithm and must, therefore, be specified. In specifying the Q and R matrices, one can initially assume that the cross-correlation coefficients are small compared to the auto correlation coefficients so that only the diagonal terms are significant in the covariance matrices. These diagonal terms correspond to the expected variances in the state and measured variables. Subsequently, cross correlations can be allowed for if, and where, expected.

Changing the Q or the R matrices in the filter does affect the filter operation considerably. Increasing Q would indicate either stronger noise driving the dynamics or increased uncertainty in the adequacy of the filter model itself to show the true dynamics accurately. This will increase the rate of growth of the elements of the P matrix. As a result, the filter gain will generally increase, thereby weighing the measurements more heavily. This is to be expected since increased Q implies that one is placing less confidence in the output of the filter's own dynamics model. By similar reasoning, increased R would indicate that the measurements are subjected to a stronger corruptive noise, and so should be weighted less by the filter. This means that the filter treats the measurements with greater reservation.

"Filter Tuning" essentially means that we have to find the reasonable values of the Q and R matrices for an effective operational filter.

VI.6 THE EXTENDED KALMAN FILTER

As mentioned in section II.4.3, most of the engineering problems are non-linear and must be linearized before the linear filter theory can be applied. Supposing that the non-linear system is described by

$$dx_t = F(x_t,u_t)dt + G(t)d\beta_t \quad \ldots\ldots\ldots\ldots \text{VI.1}$$

with discrete measurements

$$y(t_k) = h(x(t_k)) + v_{t_k} \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{VI.2}$$

where the symbols are as defined in section II.4.3.

Now consider the deterministic reference trajectory $\bar{x}_t$ and a nominal value of u_t called $\bar{u}_t$ which satisfies

$$d\bar{x}_t = F(\bar{x}_t,\bar{u}_t)dt \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{VI.3}$$

Define:

$$\delta x_t \triangleq x_t - \bar{x}_t \quad \text{and} \quad \delta u_t = u_t - \bar{u}_t \quad \ldots\ldots\ldots \text{VI.4}$$

i.e. the deviations from the reference trajectory.

We can see that δx_t is a stochastic process satisfying the differential equation

$$d(\delta x_t) = \{F(x_t,u_t) - F(\bar{x}_t,\bar{u}_t)\}dt + G(t)d\beta_t \quad \ldots\ldots\ldots\ldots \text{VI.5}$$

If the deviations from the reference trajectory are "small", then a Taylor series expansion gives

$$F(x_t u_t) - F(\bar{x}_t, \bar{u}_t) \simeq A(\bar{x}_t, \bar{u}_t).\delta x_t + D(\bar{x}_t, \bar{u}_t).\delta u_t \quad \ldots\ldots\ldots\ldots\ldots \text{VI.6}$$

where

$$A(\bar{x}_t, \bar{u}_t) = \left.\frac{\partial F_i(x_t, u_t)}{\partial x_j}\right|_{\bar{x}_t, \bar{u}_t} \quad \ldots\ldots\ldots\ldots \text{VI.7}$$

$$D(\bar{x}_t, \bar{u}_t) = \left.\frac{\partial F_i(x_t, u_t)}{\partial u_j}\right|_{\bar{x}_t, \bar{u}_t} \quad \ldots\ldots\ldots\ldots \text{VI.8}$$

Substituting from VI.6 into VI.5 we get

$$d(\delta x_t) = A(\bar{x}_t, \bar{u}_t)\delta x_t.dt + D(\bar{x}_t, \bar{u}_t)\delta u_t.dt + G(t)d\beta_t \quad \ldots\ldots\ldots\ldots \text{VI.9}$$

After integration and assuming that the deterministic system inputs are time-invariant between t_k and t_{k+1} (piecewise constant), equation VI.9 can be discretised as before

$$\delta x(t_{k+1}) = \Phi(t_{k+1}, t_k)\delta x(t_k) + \Gamma_D(t_k)\delta u(t_k) + \Gamma(t_k)w_{t_{k+1}} \quad \ldots\ldots\ldots\ldots \text{VI.10}$$

where Φ is usual state transition matrix and the rest of the symbols are as defined in section II.4.1.

By the same procedure, the measurement equation can be linearized about $\bar{x}_t$ to give

$$\delta y(t_k) = M(\bar{x}_t)\delta x(t_k) + v_{t_k} \quad \ldots\ldots\ldots\ldots \text{VI.11}$$

where

$$M(\bar{x}_t) = \left.\frac{\partial h_i(x(t_k))}{\partial x_j}\right|_{\bar{x}_t}$$

To summarize the linearized equations are:

$$\delta x(t_{k+1}) = \Phi(t_{k+1},t_k)\delta x(t_k) + \Gamma_D(t_k)\delta u(t_k) + \Gamma(t_k)w_{t_{k+1}}$$

$$\ldots\ldots\ldots\ldots\ldots \text{VI.12}$$

$$\delta y(t_k) = M(\bar{x}_t)\delta x(t_k) + v_{t_k} \quad \ldots\ldots\ldots\ldots \text{VI.13}$$

It can be seen that the linear filtering algorithm introduced in section II.4.1 is directly applicable provided that the state and measured variables are replaced by the "deviations" from a reference tragectory. Given a reference trajectory and measurements $y(t_k)$, we can then compute $\delta y(t_k)$ and process the measurement deviations through the linear filter to estimate the state deviations and then back calculate the actual state estimates.

The remaining problems are the choice of the reference trajectory and the question of the validity of the linearized equations. The obvious choice of the reference trajectory at time t_o is a priori estimate of the state. However, if the estimate is not as accurate as it should be (if $p(o,o)$ or Q is large), then the estimates of the state deviations can become large, violating the linearity assumption. In the case of a poor a priori estimate of state, it

may be worthwhile to use an iterative approach to improve on it. This means that having processed the first batch of the measurements and computed the first estimates of the state one can then predict backward to t_o using

$$\delta\hat{\underline{x}}(t_o,t_k) = \Phi(t_o,t_k)\delta\hat{\underline{x}}(t_o,t_k) + \Gamma_D(t_k)\delta\hat{\underline{u}}(t_k) \quad \text{..... VI.14}$$

Thus

$$\bar{\underline{x}}'(t_o) = \bar{\underline{x}}(t_o) + \delta\hat{\underline{x}}(t_o,t_k) \quad \text{..... VI.15}$$

If the processed batch of measurements is sufficiently large, we can expect $\bar{\underline{x}}'(t_o)$ to be closer to the "true" state than $\bar{\underline{x}}(t_o)$. This procedure can be repeated several times until no further improvement is achieved.

As an alternative, since the linear filter has a recursive structure, one can go a step further and relinearize about each last estimate as it becomes available. In other words, the reference trajectory is not fixed any longer and a better reference trajectory is used as soon as it becomes available. By this sequence of relinearization large initial estimation errors are not allowed to propogate through time and, therefore, the linearity assumptions are less likely to be violated. Here the prediction stage is accomplished by the integration of the non-linear system differential equations with the noise term equal to zero.

Some authors (16), have argued that by a sequence of relinearization one is able to process the actual

state and measured variables as opposed to the "deviations". In practice, this is possible if the measurement relationship is linear or very mildly non-linear.

Notation:

x_t	continuous variable
$x(t_k)$	discrete variable
x_k and $x(k)$	abriviations for $x(t_k)$
t	continuous time
t_k	discrete time
$\bar{x}$	the estimated value of x
$\hat{x}$	the predicted value of x

VI.7 PARAMETER ESTIMATION

Frequently, in applications, the dynamical system depends upon certain parameters whose values are imprecisely known. These parameters may be treated as pseudo state variables whose differential equations are equal to zero and thus estimated. The implication of this is that one is effectively treating the parameters as random variables and thus their a priori statistics needs to be known.

Each estimated parameter increases the dimensionality of the filter and thus the computational load. On the other hand better accuracy may result if more parameters are estimated. Therefore, some trade-off may be necessary between the number of estimated parameters and the accuracy of estimation.

An alternative approach is to take into account the effect of the parameters in degrading the estimates of the state, without estimating the parameters themselves as in the Schmidt-Kalman filter (16). However, this means that the actual filter algorithm has to be modified and thus will not be adopted in this research since it also increases the dimensionality of the filter which may not be justifiable for distillation.

VI.8 THE STATE TRANSITION MATRIX Φ

(a) Linear Systems

Consider the linear, time-varying, continuous-time system of stochastic differential equations:

$$dx_t = \mathbf{A}(t)x_t.dt + D(t)u_t.dt + G(t).d\beta_t \quad \ldots \text{ VI.16}$$

with initial conditions $x(t_o) = x_o$

Assuming $A(t)$ and $D(t)u_t$ are piecewise continuous, the solution to this equation is

$$x_t = \Phi(t,t_o)x_t + \int_{t_o}^{t} \Phi(t,\tau)D(\tau)u_\tau.d\tau + \int_{t_o}^{t} \Phi(t,\tau)G(\tau).d\beta_\tau \quad \ldots\ldots\ldots\ldots\ldots \text{ VI.17}$$

where Φ is the state transition matrix defined by

$$\frac{d\Phi(t,t_o)}{dt} = A(t)\Phi(t,t_o) \quad \ldots\ldots\ldots\ldots\ldots \text{ VI.18}$$

Significant properties of the state transition matrix include:

(i) $\Phi(t,\tau)$ is uniquely defined for all t and τ in (o,∞)

(ii) the semigroup property i.e.
$\Phi(t,\xi) = \phi(t,\tau)\Phi(\tau,\xi)$ for all t,τ and ξ

(iii) $\Phi(t,\tau)$ is non-singular and invertible:
$\Phi^{-1}(t,\tau) = \Phi(\tau,t)$

The discrete-time "equivalent" of this continuous-time model would have a solution similar to equation VI.17 with t replaced with t_k

$$\Phi(t_{k+1}) = \Phi(t_{k+1},t_k)x(t_k) + \int_{t_k}^{t_{k+1}} \Phi(t_{k+1},\tau)D(\tau)u_\tau . d\tau + \int_{t_k}^{t_{k+1}} \Phi(t_{k+1},\tau)G(\tau).d\beta$$

..... VI.19

with the state transition matrix defined as for the continuous-time system.

The two systems are "equivalent" in the sense that the discrete-time model values $x(t_1), x(t_2)....,$ are identical to those of the continuous-time at these particular times.

Schwarz and Friedland(139) by integration of equation VI.18 deduce that

$$\Phi(t,t_o) = \exp\left(\int_{t_o}^{t} A(\tau)d\tau\right) \quad \text{..... VI.20}$$

Unfortunately, however, this relation is not valid unless A(t) and $\int_{t_o}^{t} A(\tau)d\tau$ commute. One such case occurs when the matrix A(t) is the product of a constant matrix and a scalar time function, i.e.

$$\underline{A}(t) = g(t)\underline{k}$$

In this case: $\Phi(t,t_o) = \exp\left(\int_{t_o}^{t} \underline{A}(\tau)d\tau\right) = \exp\left(\underline{k}\int_{t_o}^{t} g(\tau)d\tau\right)$

..... VI.21

Amundson(140) shows that equation VI.18 can be integrated by repeated substitution to give

$$\Phi(t,t_o) = I + \int_{t_o}^{t} A(t_1)dt_1 + \int_{t_o}^{t} A(t_1)dt_1 \int_{t_o}^{t} A(t_2)dt_2 +$$

$$\int_{t_o}^{t} A(t_1)dt_1 \int_{t_o}^{t} A(t_2)dt_2$$

$$\int_{t_o}^{t} A(t_3)dt_3 + \ldots.$$

..... VI.22

Again, this integration can only be performed under special circumstances. Therefore, it remains to conclude that the evaluation of Φ in the general sense is impossible in practice.

However, if the system of differential equations is assumed to be time-invariant (A is a constant matrix), then the associated $\Phi(t,t_o)$ could be characterized further. If A is a constant matrix, then the associated $\Phi(t,t_o)$ is not a function of the separate arguments t and t_o but a function only of a single parameter $(t-t_o)$. Thus the general defining relationship for Φ reduces to

$$\frac{d}{dt}\Phi(t-t_o) = A\Phi(t-t_o); \quad \Phi(0) = I \ldots\ldots\ldots\ VI.23$$

to which the solution can be expressed as the matrix exponential

$$\Phi(t,t_o) = \Phi(t-t_o) = \exp(A\delta t); \quad \delta t = t-t_o \ldots VI.24$$

Similarly for the discrete time-model.

(b) Non-linear Systems

If the linear filter algorithm is to be applied to non-linear systems the golden rule to be followed is not to violate the linearity assumption. As shown in section VI.6, a non-linear system of stochastic differential equations can be linearized to give

$$d(\delta x_t) = A(\bar{x}_t, \bar{u}_t)\,\delta x_t.dt + D(\bar{x}_t, \bar{u}_t)\,\delta u_t.dt + G(t).d\beta_t$$

This system is identical to the linear system provided that state and measurement "deviations" are processed in the filter algorithm and the deviations are kept "small". This means that the dynamic behaviour of the non-linear system is approximated by a linear system over the time interval δt. Thus the linear filter algorithm is applicable provided that δt and thus δx and δu which are implicit functions of time are "small" enough not to violate the linearity assumption.

The state transition matrix for this linearized system can now be evaluated as if it were a linear system. Once again to make the evaluation possible, in practice, one has to assume that the system is time-invariant over the time interval δt. However, this assumption is likely to be more restrictive now. Because, if the prediction stage in the linear filter algorithm is accomplished using this approximate state transition matrix, the inaccuracies, resulting from linearization on the one hand and the assumption of

time-invariance on the other, may accumulate and violate the linearity assumption inherent in the linear filter algorithm and cause divergence. Thus it makes sense to try to avoid the use of Φ as far as possible. Φ appears in the prediction of $x(t_{k+1})$ and the covariance matrix P. The prediction of $x(t_{k+1})$ can be accomplished by the integration of the system of non-linear differential equations. As regards P, a similar approach can also be adopted in that the time propagation relation for P can be integrated. However, this integration can be cumbersome and lengthy, and, for this reason only, it is preferable to discretise the dynamics and compute P via Φ.

VI.9 PROPOSED ALGORITHM FOR THE IMPLEMENTATION OF EXTENDED KALMAN FILTERS

The following algorithm is believed to broaden the flexibility and horizons of extended Kalman filtering in process applications:

1. Set k=0 : guess $\bar{x}(t_k)$, $\bar{u}(t_k)$, p(k,k) and thus $\bar{y}(t_k)$.

2. Compute Φ based on $\bar{x}(t_k)$.

3. Predict $\hat{x}(t_{k+1})$ by the integration of the non-linear differential equations (filter model) starting from $\bar{x}(t_k)$.

4. Compute the predicted state and measurement deviations using

$$\delta\hat{x}(t_{k+1}) = \hat{x}(t_{k+1}) - \bar{x}(t_k)$$

$$\delta y(t_{k+1}) = y(t_{k+1}) - \bar{y}(t_k)$$

5. Process the deviations through the linear filter algorithm introduced in Section II.4.2 and thus produce $\delta\bar{x}(t_{k+1})$.

6. Compute $\bar{x}(t_{k+1})$ using $\bar{x}(t_{k+1}) = \delta\bar{x}(t_{k+1}) + \bar{x}(t_k)$.

7. Compute $\bar{y}(t_{k+1})$ using the filter model or otherwise.

8. Set k=k+1, return to step 2 and continue.

C H A P T E R S E V E N

THE ESTIMATORS AND SIMULATED OPEN-LOOP ESTIMATION RESULTS

VII.1 THE FILTERS FORMULATED

The extended Kalman filters formulated have the following common features:

(i) use Model I discussed in Chapter IV as the filter's system model. It is worth noting that Model I is highly simplified and inaccurate compared with the column simulator model (Model II, Chapter IV).

(ii) Compute the state transition matrix via

$$\Phi(k+1,k) = I + \frac{\partial f(x_k,u_k)}{\partial x_k}.\delta t \quad \ldots\ldots\ldots\ldots \text{VII.1}$$

where δt is the sample time and the jacobian $\frac{\partial f(x_k,u_k)}{\partial x_k}$ is evaluated about the latest estimated state

(iii) a sample time of 18 seconds

(iv) the initial estimate of the state is provided by an approximate McCabe-Thiele calculation

The estimation simulation studies are carried out using the process simulator (Model II, Chapter IV) which has already been shown to represent the dynamic and static characters of the distillation column with reasonable accuracy (see Chapter V). The filters formulated and the associated filter models are simply inserted into the simulator with the necessary channels for the inter-communications. The filtering philosophy is then implemented as depicted in Figure VI.1, while the algorithm given in Section VI.9 helps provide

better insight into the precedural completion of the various steps involved. The additional programs needed essentially include a library of matrix and vector manipulation routines and a subroutine for the initialization of the filter model. Once again the programs are largely self-documenting and the listings shown in Appendix E should provide enough information for the programs to be followed. Therefore, detailed discussion of the individual subroutines will be foregone. However, some elaboration on the main program arrangement may be in order at this stage.

VII.2 FILTERING SIMULATION PACKAGE : THE MAIN PROGRAM SEGMENTS

The main segments of the simulation package for estimation are:

SUBROUTINE INDATA - Read in the data required for the initialization of the column simulator based on Model II, plus the details of the deterministic disturbances to be introduced and P,R and Q matrices.

SUBROUTINE HKEEP - Subroutine to calculate the Antoine and Van Laar constants.

SUBROUTINE SDWEG - Subroutine to find the reflux ratio for a desired separation by Wegstein algorithm.

SUBROUTINE SSMODL - Subroutine to perform McCabe-Thiele calculation for the initialization of the column simulator and filter model.

SUBROUTINE GOFIL - Subroutine to initialize the column simulator and the filter model.

SUBROUTINE LATEST - Subroutine to compute Φ and store the latest estimated state and measured variables.

SUBROUTINE DISCOL - The column simulator subroutine.

SUBROUTINE SIMUL - The filter model.

SUBROUTINE PRINT - Subroutine to print out variables of interest.

SUBROUTINE SDBUB - Bubble point calculation.

SUBROUTINE SDDEW - Dew point calculation.

SUBROUTINES SDINT, INTJS and INTPAS - Subroutines constituting the SDINT integrator.

SUBROUTINE EFF - Efficiency calculation.

SUBROUTINE MATINV - Matrix inversion by Gauss-Jordan elimination.

SUBROUTINE MATTPS - Matrix transposition.

SUBROUTINE MATMUL - Matrix multiplication.

SUBROUTINE MATADD - Matrix addition.

SUBROUTINE MATSUB - Matrix subtraction.

SUBROUTINE MATVEC - Matrix-vector multiplication.

SUBROUTINE VECADD - Vector addition.

SUBROUTINE VECSUB - Vector subtraction.

SUBROUTINE Kalman - The filter.

The package also contains a number of other sub-routines that essentially facilitate the communication with the package and whose listings should be self-explanatory (see Appendix E) (Microfiche).

The flow chart for the main program arrangement is shown in VII.1. The filters tested in this research are:

Extended Kalman Filter 1 (EKF1) : State estimation from noisy tray composition measurements.

Extended Kalman Filter 2 (EKF2) : State estimation from noisy tray temperature measurements.

Extended Kalman Filter 3 (EKF3) : State and parameter estimation from noisy tray temperature measurements.

These filters will now be described in more detail.

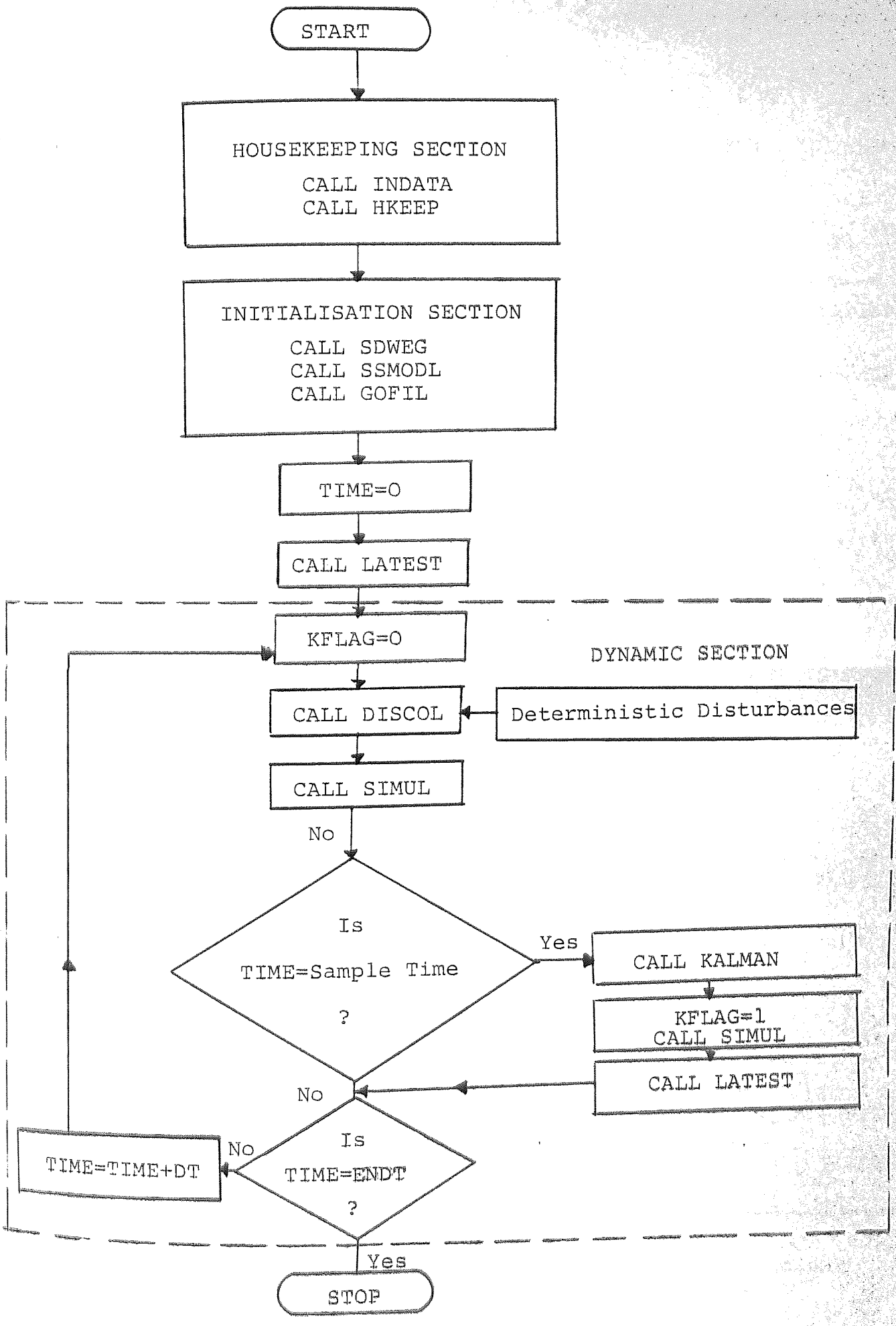


FIGURE VII.1 - The Main Program Arrangement for the Filtering Package

N.B. If KFLAG=1, the filter model bypasses the Integration Section

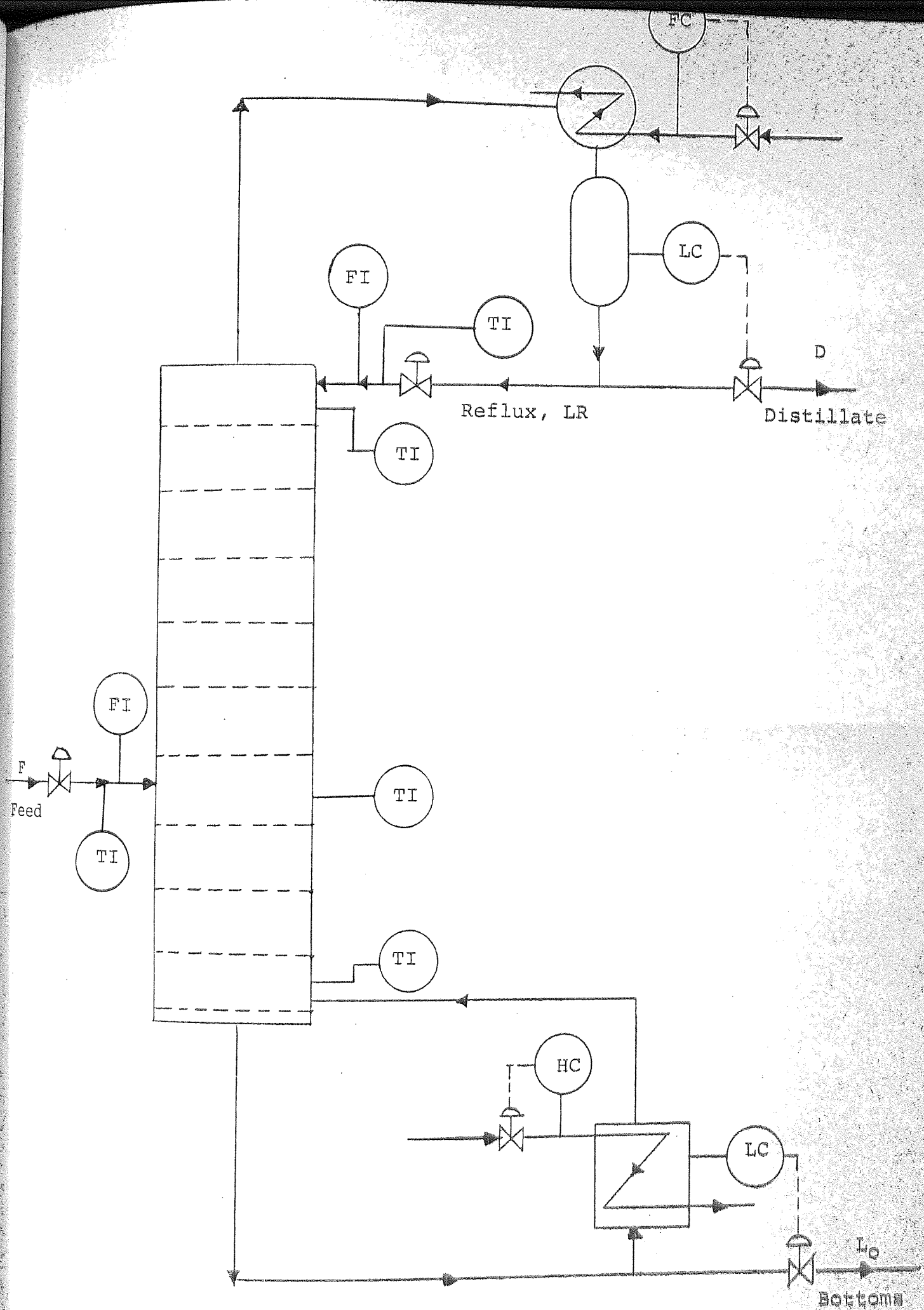


Figure VII.2 - The Symbolic Representation of the Column Used for Open-Loop Estimation

VII.3 STATE ESTIMATION FROM NOISY COMPOSITION MEASUREMENTS : EKF1

The symbolic representation of the column used for open-loop estimation is depicted in Figure VII.2.

VII.3.1 THE STATE VARIABLES

Since the symbol x is used to denote the state variables in the filter algorithm and also the mole fraction of the M.V.C. on the nth tray, the following notation will be used to avoid confusion:

x_j denotes the state variables

x_n denotes the mole fraction of the M.V.C. on the nth tray

M_n denotes the liquid holdup on the nth tray

i.e. variables subscripted by n refer to the mole fractions and those subscripted by j denote the state variables.

The elements of the state vector are:

$$x_j = x_n \qquad j = 1,11;\ n = 1,11$$

$$x_j = M_n \qquad j = 11,22;\ n = 1,11$$

VII.3.2 THE STATE TRANSITION MATRIX (22-by-22)

In equation VII.1 the Jacobian $\frac{\partial f(x_k, u_k)}{\partial x_k}$ will henceforth be abbreviated to $\frac{\partial f}{\partial x}$ for convenience of notation. $\frac{\partial f}{\partial x}$ is defined as

$$\frac{\partial f}{\partial x} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_m} \end{bmatrix} \quad \ldots\ldots\ldots \text{VII.2}$$

where

$$f_1 = \frac{L_R(x_D - x_1) + v(y_2 - y_1)}{M_1}$$

$$f_i = \frac{L_{i-1}(x_{i-1} - x_i) + v(y_{i+1} - y_i)}{M_i} \quad ; \quad i=2,6$$

$$f_7 = \frac{L_6(x_6 - x_7) + v(y_8 - y_7) + F(x_F - x_7)}{M_7}$$

$$f_i = \frac{L_{i-1}(x_{i-1} - x_i) + v(y_{i+1} - y_i)}{M_i} \quad ; \quad i=8,10$$

$$f_{11} = \frac{L_{10}(x_{10} - x_{11}) + v(x_{11} - y_{11})}{M_{11}}$$

$$f_{12} = L_R - L_1$$

$$f_i = L_{i-11} - L_{i-12} \quad ; \quad i=13,17$$

N.B. During the partial differentiation of $f_i (i=1,11)$ with respect to the liquid composition, for simplicity, the functional relationship between y_i and $x_i (i=1,11)$ has been ignored. This may be considered as a modelling error and from reported experience the filters should be insensitive to these types of errors. Had this functional relationship been included, the corresponding elements of the state transition matrix would have been modified as illustrated in Appendix G.

$$f_{18} = L_6 - L_7 + F$$

$$f_i = L_{i-11} - L_{i-12}; \quad i=19,21$$

$$f_{22} = L_{10} - L_{11} - v$$

The rows of the Jacobian can now be calculated as follows:

First Row

$$\frac{\partial f_1}{\partial x_1} = -\frac{L_R}{M_1}$$

$$\frac{\partial f_i}{\partial x_j} = 0; \quad j=2,11$$

$$\frac{\partial f_1}{\partial x_{12}} = \frac{-\{L_R(x_D-x_1) + v(y_2-y_1)\}}{(M_1)^2}$$

$$\frac{\partial f_1}{\partial x_j} = 0; \quad j=13,22$$

Second Row

$$\frac{\partial f_2}{\partial x_1} = \frac{L_1}{M_2}$$

$$\frac{\partial f_2}{\partial x_2} = -\frac{L_1}{M_2}$$

$$\frac{\partial f_2}{\partial x_j} = 0; \quad j=3,12$$

$$\frac{\partial f_2}{\partial x_{13}} = \frac{-\{L_1(x_1-x_2) + v(y_3-y_2)\}}{(M_2)^2}$$

$$\frac{\partial f_2}{\partial x_j} = 0; \quad j=14,22$$

Third Row

$$\frac{\partial f_3}{\partial x_1} = 0$$

$$\frac{\partial f_3}{\partial x_2} = \frac{L_2}{M_3}$$

$$\frac{\partial f_3}{\partial x_3} = -\frac{L_2}{M_3}$$

$$\frac{\partial f_3}{\partial x_j} = 0; \quad j=4,13$$

$$\frac{\partial f_3}{\partial x_{14}} = \frac{-\{L_2(x_2-x_3) + v(y_4-y_3)\}}{(M_3)^2}$$

$$\frac{\partial f_3}{\partial x_j} = 0; \quad j=15,22$$

Fourth Row

$$\frac{\partial f_4}{\partial x_j} = 0; \quad j=1,2$$

$$\frac{\partial f_4}{\partial x_3} = \frac{L_3}{M_4}$$

$$\frac{\partial f_4}{\partial x_4} = -\frac{L_3}{M_4}$$

$$\frac{\partial f_6}{\partial x_j} = 0; \quad j=7,16$$

$$\frac{\partial f_6}{\partial x_{17}} = \frac{-\{L_5(x_5-x_6) + v(y_7-y_6)\}}{(M_6)^2}$$

$$\frac{\partial f_6}{\partial x_j} = 0; \quad j=18,22$$

Seventh Row

$$\frac{\partial f_7}{\partial x_j} = 0; \quad j=1,5$$

$$\frac{\partial f_7}{\partial x_6} = \frac{L_6}{M_7}$$

$$\frac{\partial f_7}{\partial x_7} = -\frac{(L_6+F)}{M_7}$$

$$\frac{\partial f_7}{\partial x_j} = 0; \quad j=8,17$$

$$\frac{\partial f_7}{\partial x_{18}} = \frac{-\{L_6(x_6-x_7) + v(y_8-y_7) + F(x_F-x_7)\}}{(M_7)^2}$$

$$\frac{\partial f_7}{\partial x_j} = 0; \quad j=19,22$$

Eighth Row

$$\frac{\partial f_8}{\partial x_j} = 0; \quad j=1,6$$

$$\frac{\partial f_8}{\partial x_7} = \frac{L_7}{M_8}$$

$$\frac{\partial f_8}{\partial x_8} = -\frac{L_7}{M_8}$$

$$\frac{\partial f_8}{\partial x_j} = 0; \quad j=9,18$$

$$\frac{\partial f_8}{\partial x_{19}} = \frac{-\{L_7(x_7-x_8) + v(y_8-y_7)\}}{(M_8)^2}$$

$$\frac{\partial f_8}{\partial x_j} = 0; \quad j=20,22$$

Ninth Row

$$\frac{\partial f_9}{\partial x_j} = 0; \quad j=1,7$$

$$\frac{\partial f_9}{\partial x_8} = \frac{L_8}{M_9}$$

$$\frac{\partial f_9}{\partial x_9} = -\frac{L_8}{M_9}$$

$$\frac{\partial f_9}{\partial x_j} = 0; \quad j=10,19$$

$$\frac{\partial f_9}{\partial x_{20}} = \frac{-\{L_8(x_8-x_9) + v(y_{10}-y_9)\}}{(M_9)^2}$$

$$\frac{\partial f_9}{\partial x_j} = 0; \quad j=21,22$$

Tenth Row

$$\frac{\partial f_{10}}{\partial x_j} = 0; \quad j=1,8$$

$$\frac{\partial f_{10}}{\partial x_9} = \frac{L_9}{M_{10}}$$

$$\frac{\partial f_{10}}{\partial x_{10}} = -\frac{L_9}{M_{10}}$$

$$\frac{\partial f_{10}}{\partial x_j} = 0; \quad j=11,20$$

$$\frac{\partial f_{10}}{\partial x_{21}} = \frac{-\{L_9(x_9-x_{10}) + v(y_{11}-y_{10})\}}{(M_{10})^2}$$

$$\frac{\partial f_{10}}{\partial x_{22}} = 0$$

Eleventh Row

$$\frac{\partial f_{11}}{\partial x_j} = 0; \quad j=1,9$$

$$\frac{\partial f_{11}}{\partial x_{10}} = \frac{L_{10}}{M_{11}}$$

$$\frac{\partial f_{11}}{\partial x_{11}} = \frac{-L_{10} + v}{M_{11}}$$

$$\frac{\partial f_{11}}{\partial x_j} = 0; \quad j=12,21$$

$$\frac{\partial f_{11}}{\partial x_{22}} = \frac{-\{L_{10}(x_{10}-x_{11}) + v(x_{11}-y_{11})\}}{(M_{11})^2}$$

Twelfth to Twenty Second Rows

$$\frac{\partial f_i}{\partial x_j} = 0; \quad i=12,22; \; j=1,22$$

Thus having computed the Jacobian, the calculation of Φ is a mere formality.

VII.3.3 THE MEASUREMENT VECTOR (3-by-1)

Assuming three composition measurements are available, the measurement vector donated by y consists of:

$y_1 = x_1$: liquid composition on the topmost tray

$y_2 = x_7$: liquid composition on the feed tray

$y_3 = x_{10}$: liquid composition on the lowermost tray

VII.3.4 THE MEASUREMENT MATRIX (3-by-22)

The elements of the measurement matrix are all zero except:

M(1,1) = 1.0

M(2,7) = 1.0

M(3,10) = 1.0

VII.3.5 THE MEASUREMENT NOISE MATRIX (3-by-3)

The non-diagonal elements of this matrix are zero. The diagonal elements were chosen to be:

R = diag. {0.003 0.003 0.003}

This means that the standard deviation of the composition measurements is 5.4%.

VII.3.6 THE SYSTEM NOISE MATRIX (22-by-22)

The non-diagonal elements of this matrix are also zero. The diagonal elements were all selected as 0.003 which is the average expected value obtained by comparison of the predictions of Model I (the filter model) with Model II (the column simulator model) in Chapter V, i.e.

Q = diag. {0.003 ..... 0.003}

VII.3.7 THE INITIAL ERROR COVARIANCE MATRIX (22-by-22)

The non-diagonal elements of the P(0,0) matrix are set to zero. The diagonal elements are all equal to 0.001, i.e.

P(0,0) = diag. {0.001 ..... 0.001}

This means that the standard deviation of the initial composition estimates is 3.1% while that of the holdups is 31%. i.e. we have less confidence in our initial estimates of the holdups.

VII.3.8 THE INITIAL ESTIMATE OF THE STATE

This is calculated internally by the simulator by a McCabe-Thiele calculation for the separation

$F = 10$ mole/hr.

$x_F = 0.4$

$x_D = 0.91$

$x_B = 0.09$

$R = 2.0$

Having calculated the compositions and the rates, the tray hold-ups are then calculated internally using the truncated Brambilla correlation.

VII.3.9 THE SIMULATED MEASUREMENT NOISE

The composition measurements were corrupted by a white Gaussian noise characterized by $(0, \sqrt{0.003})$ which was added to the composition measurements.

VII.3.10 THE SIMULATION RESULTS USING EKF1

The simulation studies in Chapter V show that starting from an approximate steady-state predicted by the McCabe-Thiele's method, the column simulator undergoes a transient period to reach a more accurate steady-state. The state estimates produced by EKF1 during this transient period continued to track the actual state through to the refined steady-state with excellent accuracy. The maximum estimation error as regards the tray compositions was in the order of 0.004 and much less for the holdups. Even when step

disturbances were introduced into the column at steady-state which were "unknown" to the filter and its model, the estimates still continued to track the actual states with a comparable accuracy. The following "unknown" disturbances were studied in this context:

(i) 10% step changes in the feed rate and composition

(ii) 10% step changes in the boilup and reflux rates

(iii) 10% step changes in the feed and reflux stream temperatures

In all these case studies, the filter showed no difficulty in producing accurate estimates of the tray compositions and holdups. It was then decided to use simple Euler for the integration of the filter model equations while the column simulator used the fourth-order Runge-Kutta with the same step size and the sample time was increased to 36 seconds. Here, again, the filter exhibited no difficulty in estimating the tray compositions and holdups. This can be a valuable feature because it can reduce the calculation cycle time considerably and the advantage of being able to increase the sample time is always desirable - especially in high dimensionality systems.

Another interesting feature of EKF1 was that, with a sample time of 18 seconds only, it was possible to process the actual state and measured variables through the filter as opposed to the deviations from the latest estimated trajectory. This is because the

measurement functional relationship is linear and the filter is apparently capable of coping with the non-linearities due to the system model with a small sample time.

It remains to conclude that the simulation studies using EKF1 were sufficiently encouraging to proceed to explore the additional capabilities of the extended Kalman filter in application to distillation columns.

VII.4 STATE ESTIMATION FROM NOISY TRAY TEMPERATURE MEASUREMENTS : EKF2

The state vector and the state transition matrix for this filter are identical to the EKF1.

VII.4.1 THE MEASUREMENT VECTOR (3-by-1)

The measurement vector consists of:

$y_1 = T_1$: the topmost tray temperature

$y_2 = T_7$: the feed tray temperature

$y_3 = T_{10}$: the lowermost tray temperature

VII.4.2 THE MEASUREMENT MATRIX (3-by-22)

Since the state variables are not being measured directly, a functional relationship is needed to relate the measured variables to the state variables, i.e. $T = g(x)$. Moreover, this function has to be continuous and differentiable. For a binary mixture it can be shown that on each tray

$$x_1 = \frac{P - P_2^o(T)}{P_1^o(T) - P_2^o(T)} \qquad \text{..... VII.2}$$

Using the following physical laws:

(i) Raoult's law : $x_i P_i^o(T) = P_i$

(ii) Dalton's law : $P_i = y_i P$

(iii) Antoine's equation : $\log P_i^o(T) = A_i - \frac{B_i}{C_i+T}$

where

x_i, y_i = liquid and vapour mole fractions of component i

P_i = partial pressure of component i (mm. Hg.)

$P_i^o(T)$ = vapour pressure of i (mm. Hg.)

P = total system pressure (mm. Hg.)

For convenience of differentiation since T is a function of x only in this particular case we can write

$$\frac{\partial T}{\partial x} = \frac{1}{\frac{\partial x}{\partial T}} = \frac{\{P_1^o(T) - P_2^o(T)\}^2}{-\frac{\partial P_2^o}{\partial T}\{P_1^o(T) - P_2^o(T)\} - \{\frac{\partial P_1^o(T)}{\partial T} - \frac{\partial P_2^o(T)}{\partial T}\}\{P - P_2^o(T)\}} \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{VII.3}$$

where

$$\frac{\partial P_i^o(T)}{\partial T} = \frac{2.303 B_i}{(C_i+T)^2} P_i(T)$$

The measurement matrix is therefore a matrix of zero elements except

$$M(1,1) = \frac{\partial T_1}{\partial x_1}$$

$$M(2,7) = \frac{\partial T_7}{\partial x_7}$$

$$M(3,10) = \frac{\partial T_{10}}{\partial x_{10}}$$

VII.4.3 THE MEASUREMENT NOISE MATRIX (3-by-3)

$$R = \text{diag.}\{0.01 \quad 0.01 \quad 0.01\}$$

The figure 0.01 is, in actuality, the expected variance about the regression plane of one of the thermocouples on the column.

VII.4.4 THE SYSTEM NOISE MATRIX (22-by-22)

The diagonal elements of Q were found by trial and error starting from the average expected variance 0.003, obtained by comparison of Models I and II, in Chapter V.

$$Q = \text{diag.}\{0.006, 0.009, 0.009, 0.09, 0.09, 0.006 \ldots 0.006\}$$

VII.4.5 THE INITIAL ERROR COVARIANCE MATRIX : 22-by-22

This is the same as EKFI

$$P(0,0) = \text{diag.}\{0.001 \ldots\ldots\ldots\ldots\ldots\ldots 0.001\}$$

VII.4.6 THE INITIAL ESTIMATE OF THE STATE

This is calculated in a similar manner to EKFI.

VII.4.7 THE SIMULATED MEASUREMENT NOISE

The temperature measurements are corrupted by a white Gaussian sequence characterized by $(0, \sqrt{0.01})$ which is added to the temperature measurements. Notice that the size of the noise should not exceed what we have allowed for through the R matrix.

VII.5 STATE AND PARAMETER ESTIMATION FROM NOISY TRAY TEMPERATURE MEASUREMENTS: EKF3

The system inputs which are of primary importance in the study of dynamics and control of binary distillation columns are namely:

(i) the feed rate : F

(ii) the feed composition : x_F

(iii) the reflux rate : L_R

(iv) the boilup rate : v

Admittedly other inputs could also be considered. However, since every estimated input increases the dimensionality of the filter and thus the inter-sample computational load, each input must be selected judiciously according to its merits and influence on the predictions of the filter model. As regards binary distillation columns, it is difficult to justify other inputs outside the ones listed above. The EKF3 estimates these inputs by treating them as pseudo state variables with their differential equations equal to zero.

VII.5.1 THE STATE VECTOR (26-by-1)

The first 24 elements of the state vector are the same as EKF1. The last 4 elements are

$x_{23} = F$ $\qquad$ $x_{25} = v$

$x_{24} = x_F$ $\qquad$ $x_{26} = L_R$

VII.5.2 THE STATE TRANSITION MATRIX (26-by-26)

The Jacobian in the state transition matrix is much the same as EKF1 except for the following additional non-zero elements which correspond to the additional four pseudo state variables in the state vector.

First Row

$$\frac{\partial f_1}{\partial x_{25}} = \frac{y_2 - y_1}{M_1}$$

$$\frac{\partial f_1}{\partial x_{26}} = \frac{x_D - x_1}{M_1}$$

Second Row

$$\frac{\partial f_2}{\partial x_{25}} = \frac{y_3 - y_2}{M_2}$$

Third Row

$$\frac{\partial f_3}{\partial x_{25}} = \frac{y_4 - y_3}{M_3}$$

Fourth Row

$$\frac{\partial f_4}{\partial x_{25}} = \frac{y_5 - y_4}{M_4}$$

Fifth Row

$$\frac{\partial f_5}{\partial x_{25}} = \frac{y_6 - y_5}{M_5}$$

Sixth Row

$$\frac{\partial f_6}{\partial x_{25}} = \frac{y_7 - y_6}{M_6}$$

Seventh Row

$$\frac{\partial f_7}{\partial x_{23}} = \frac{x_F - x_7}{M_7}$$

$$\frac{\partial f_7}{\partial x_{24}} = \frac{F}{M_7}$$

$$\frac{\partial f_7}{\partial x_{25}} = \frac{y_8 - y_7}{M_7}$$

Eighth Row

$$\frac{\partial f_8}{\partial x_{25}} = \frac{y_9 - y_8}{M_8}$$

Ninth Row

$$\frac{\partial f_9}{\partial x_{25}} = \frac{y_{10} - y_9}{M_9}$$

Tenth Row

$$\frac{\partial f_{10}}{\partial x_{25}} = \frac{y_{11} - y_{10}}{M_{10}}$$

Eleventh Row

$$\frac{\partial f_{11}}{\partial x_{25}} = \frac{x_{11} - y_{11}}{M_{11}}$$

Twelfth Row

$$\frac{\partial f_{12}}{\partial x_{26}} = 1.0$$

Eighteenth Row

$$\frac{\partial f_{18}}{\partial x_{23}} = 1.0$$

Twenty Second Row

$$\frac{\partial f_{22}}{\partial x_{25}} = -1.0$$

VII.5.3 THE MEASUREMENT VECTOR (5-by-1)

Since flow rate measurements can be assumed to be readily available, EKF3 expects the feed and reflux rates as measured variables. This is essentially to prevent the system from becoming unobservable which may stem from the attempted identification of a high dimensionality system from a handful of three temperature measurements. Therefore, the measurement vector consists of

$y_1 = T_1$: the topmost tray temperature

$y_2 = T_7$: the feed tray temperature

$y_3 = T_{10}$: the lowermost tray temperature

$y_4 = F$: the feed rate

$y_5 = LR$: the reflux rate

VII.5.4 THE MEASUREMENT MATRIX (5-by-26)

As in EKF2 we can write $x = g(T)$ and hence obtain $\frac{\partial T}{\partial x}$ on each tray. Thus, the elements of the measurement

matrix are all zero except

$$M(1,1) = \frac{\partial T_1}{\partial x_1}$$

$$M(2,7) = \frac{\partial T_7}{\partial x_7}$$

$$M(3,10) = \frac{\partial T_{10}}{\partial x_{10}}$$

$$M(4,23) = 1.0$$

$$M(5,26) = 1.0$$

VII.5.5 THE MEASUREMENT NOISE MATRIX (5-by-5)

$$R = \text{diag.}\{0.01 \quad 0.01 \quad 0.01 \quad 1.0 \quad 1.0\}$$

Notice this means that the standard deviation of the feed rate measurement is 10% and that of the reflux measurement is about 16%.

VII.5.6 THE SYSTEM NOISE MATRIX (26-by-26)

Once again the diagonal elements of Q were found by trial and error.

$$Q = \text{diag.}\{0.006, 0.009, 0.009, 0.09, 0.09, 0.006 \ldots\ldots 1.0, 0.15, 1.0, 1.0\}$$

VII.5.7 THE INITIAL ERROR COVARIANCE MATRIX(26-by-26)

$P(0,0) = \{0.001 \ldots\ldots\ldots 0.04\ 0.04\ 0.04\ 0.04\}$

VII.5.8 THE INITIAL ESTIMATE OF THE STATE

This is computed in a similar manner to EKF1.

VII.5.9 SIMULATED MEASUREMENT NOISE

The temperature measurements are corrupted by a white Gaussian sequence characterized by $(0,\sqrt{0.01})$. The feed rate measurement is corrupted by $(0.25,\sqrt{0.5})$ or $(0,\sqrt{0.5})$ and the reflux measurement is corrupted by $(0,\sqrt{0.4})$

VII.6 THE SIMULATION RESULTS USING EKF3

The graphical presentation of the simulation results using EKF3 will now follow. The deterministic disturbances of both known and unknown natures which were introduced simultaneously after the column had reached steady state (0.5 hrs) were:

(i) multiple step changes in the feed rate which is available to the filter as a highly corrupted measured variable (see Figure VII.8)

(ii) a ramp change followed by multiple step changes in the feed composition which is supplied to the filter as a parameter to be estimated (see Figure VII.9)

(iii) a step increase of 10°C in the feed temperature which is unknown to the filter

The steady-state filter gain is given in Table VII.1. The sample time used was 18 seconds. This filter was also tested using a sample time of 36 seconds and using simple Euler for predictions while the column simulator was being integrated by the fourth-order Runge-Kutta method - the step sizes being the same. Under these conditions and with the same input disturbances as described above, the filter was stable and the estimation was almost equally accurate.

VII.6.1 OBSERVATIONS FROM THE STEADY-STATE FILTER GAIN MATRIX : TABLE VII.1

The filter gains at the measurement points have been marked by *. It can be seen that the filter pays more attention to the state variables whose associated temperatures are being measured. The composition estimates (rows 1-11) and the boilup rate (element (25,3)) which is estimated as a pseudo state variable, benefit more from the temperature measurements than the flow measurements. It is significant that the tray holdup estimates are also weighted towards the temperature measurements except on trays 1 and 7 where feed and reflux streams enter the column (see the underlined elements). Since these are available to the filter as measured parameters which are to be estimated, the filter takes their respective measurements more into account. This is a good example of how state estimation can benefit from more estimated parameters.

VII.6.2 REMARKS ON THE ESTIMATION RESULTS

Figure VII.3:

The simulated actual and estimated liquid compositions on tray 1 where a corrupt temperature measurement is taken. The picture is slightly distorted because the plotter attempts to fit

a curve to the points. Nevertheless the estimates show remarkable agreement with the actual values.

Figure VII.4:

An example of the simulated actual and estimated liquid compositions on a tray in the enriching section where there is no measurement. The estimates are still very accurate.

Figure VII.5:

Simulated actual and estimated liquid compositions on the feed tray where a corrupt temperature measurement is taken. The points are joined by straight lines. A good demonstration of the accuracy of the estimates.

Figure VII.6:

Simulated actual and estimated liquid compositions on a tray in the stripping section where there is no temperature measurement. By contrast with plate 4, the estimates on this plate show relatively closer agreement with the actual values. This is because there are more temperature measurements in the stripping section than the enriching section.

Figure VII.7:

Simulated actual and estimated bottoms composition. There is little variation in the actual composition because of the excessively large reboiler holdup. The estimates are again accurate.

Figure VII.8:

Simulated multiple step changes in the feed rate which is supplied to the filter as a noisy measurement and the estimates produced. Although non-zero mean noise has been deliberately added to the measurements which effectively acts as a bias, the filter still tracks the development of the actual value. It is significant that although the filter is not troubled by this bias globally in that the state estimates are accurate, it is unable to remove the bias locally. i.e. the estimates of the feed rate have a distinct positive bias. This is to be expected since this type of Kalman filter is not geared to remove biases (39).

Figure VII.9:

Simulated changes in the feed composition which is available to the filter as an unmeasured parameter to be estimated. Once again there is a distinct positive bias in the estimates. It is possible that this is due to the filter

bieng unable to remove the bias in the feed flow rate estimates. Biases can also stem from non-linearities which can arise at the feed point in a distillation column.

* -.4542E-Ø1	-.5ØØ6E-Ø8	-.1638E-Ø6	-.134ØE-1Ø	.5363E-Ø6
-.8364E-Ø4	.1259E-Ø5	-.18ØØE-Ø3	-.72Ø4E-Ø8	-.2679E-Ø6
-.8Ø27E-Ø4	-.863ØE-Ø4	-.4521E-Ø3	-.2246E-Ø6	-.4454E-Ø6
-.1299E-Ø3	-.1585E-Ø2	-.7517E-Ø3	-.3861E-Ø5	-.71Ø2E-Ø6
-.1834E-Ø3	-.5569E-Ø2	-.1Ø84E-Ø2	-.14Ø5E-Ø4	-.1ØØ3E-Ø5
-.2417E-Ø3	-.3241E-Ø2	-.144ØE-Ø2	-.1Ø43E-Ø4	-.1322E-Ø5
-.3963E-Ø8	* -.36Ø7E-Ø1	-.1428E-Ø7	.1711E-Ø7	-.1768E-1Ø
-.1218E-Ø3	-.3771E-Ø4	-.2726E-Ø3	-.8Ø32E-Ø7	-.63Ø1E-Ø6
-.3266E-Ø3	-.3586E-Ø4	-.1741E-Ø2	-.1165E-Ø6	-.1723E-Ø5
-.9426E-Ø7	-.1Ø38E-Ø7	*-.2622E-Ø1	-.3ØØ1E-1Ø	-.5Ø33E-Ø9
-.1444E-Ø4	-.3879E-Ø7	-.9Ø29E-Ø4	-.674ØE-Ø9	-.7885E-Ø7
-.5435E-Ø2	-.1138E-Ø5	.2Ø22E-Ø3	-.1753E-Ø8	.1864E-Ø2
-.1317E-Ø5	-.24Ø5E-Ø3	-.8538E-Ø5	-.3721E-Ø6	-.7449E-Ø8
.1Ø76E-Ø6	-.3Ø86E-Ø4	.5649E-Ø6	-.975ØE-Ø7	.5773E-Ø9
.6365E-Ø7	-.6614E-Ø4	.3Ø76E-Ø6	-.1463E-Ø6	.321ØE-Ø9
.3994E-Ø6	-.3117E-Ø3	.1756E-Ø5	-.7694E-Ø6	.2Ø25E-Ø8
-.1326E-Ø6	.1267E-Ø3	.2323E-Ø6	.7Ø73E-Ø6	-.5121E-Ø9
-.1658E-Ø6	-.4Ø79E-Ø2	-.4626E-Ø5	.19Ø2E-Ø2	-.2837E-Ø8
-.8Ø18E-Ø5	.512ØE-Ø5	-.3571E-Ø2	.1356E-Ø7	-.5974E-Ø7
-.5531E-Ø4	.2Ø49E-Ø5	-.5688E-Ø2	.3333E-Ø9	-.3318E-Ø6
.1834E-Ø3	.3Ø26E-Ø4	-.1944E-Ø1	.8Ø38E-Ø7	.9429E-Ø6
-.9Ø97E-Ø3	.8772E-Ø5	-.579ØE-Ø2	-.1168E-Ø7	-.4949E-Ø5
.294ØE-Ø7	-.4742E-Ø4	.1144E-Ø6	* .518Ø	.139ØE-Ø9
.24ØØE-Ø3	-.6392E-Ø1	.1365E-Ø2	-.1739E-Ø3	.1292E-Ø5
.2468E-Ø1	.3785E-Ø2	.1244	.1Ø13E-Ø4	.1278E-Ø3
-.1177E-Ø2	.49ØØE-Ø7	.1919E-Ø5	.139ØE-Ø9	* .618Ø

Table VII.1
The Steady-State Filter Gain for EKF3

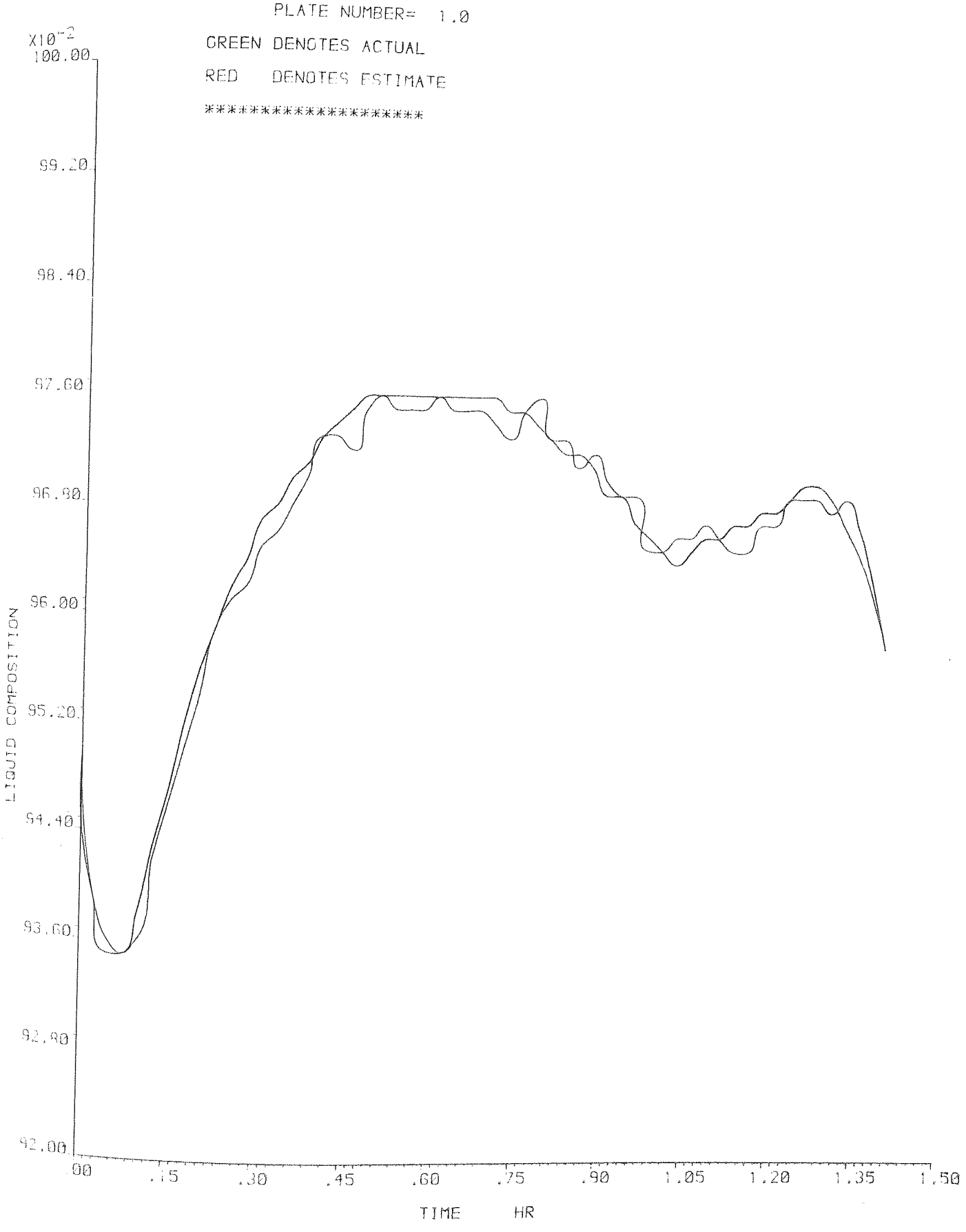


Figure VII.3
Simulated actual and estimated liquid compositions on tray 1 where a corrupt temperature measurement is taken

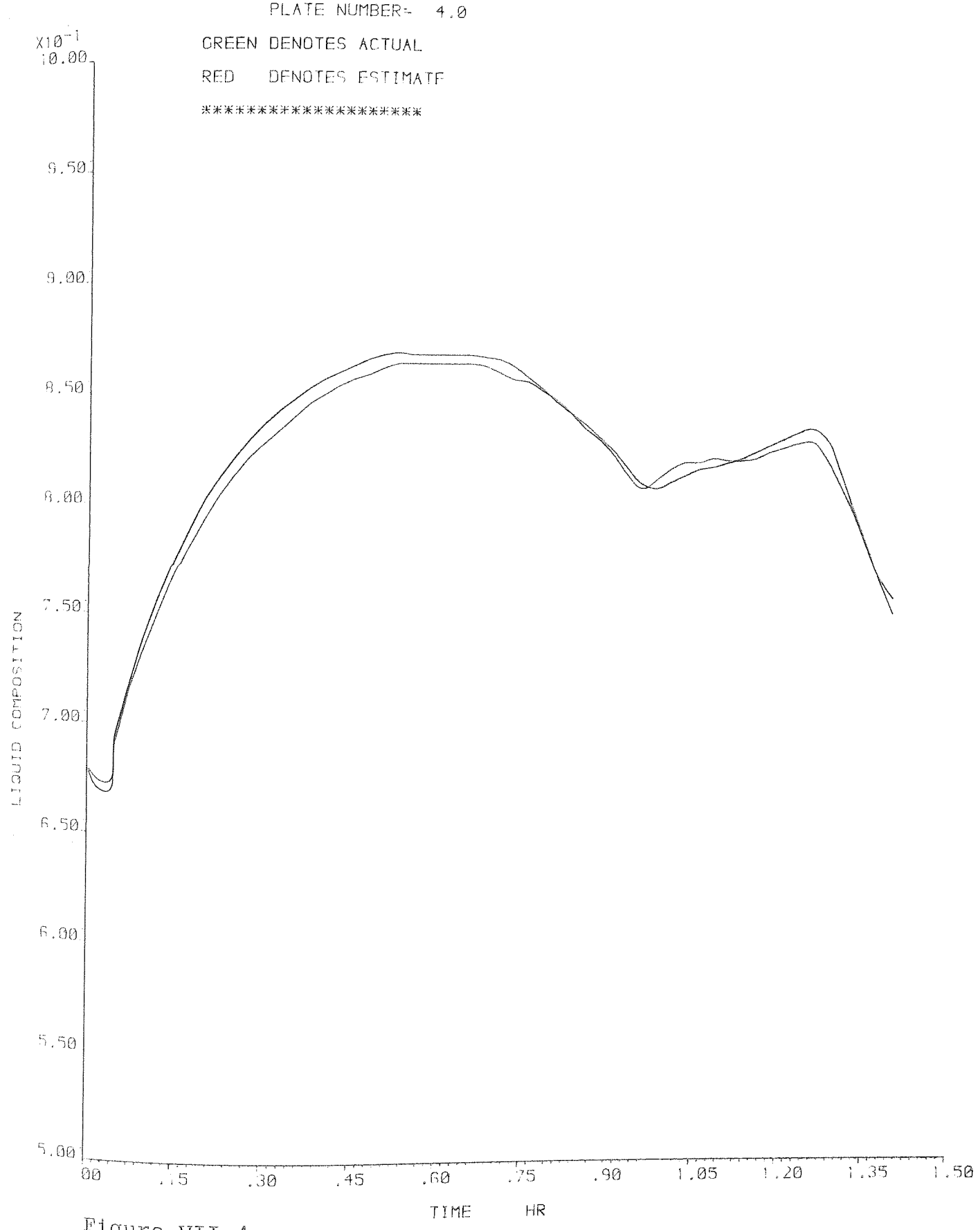


Figure VII.4
Simulated and actual liquid compositions on a tray in the enriching section

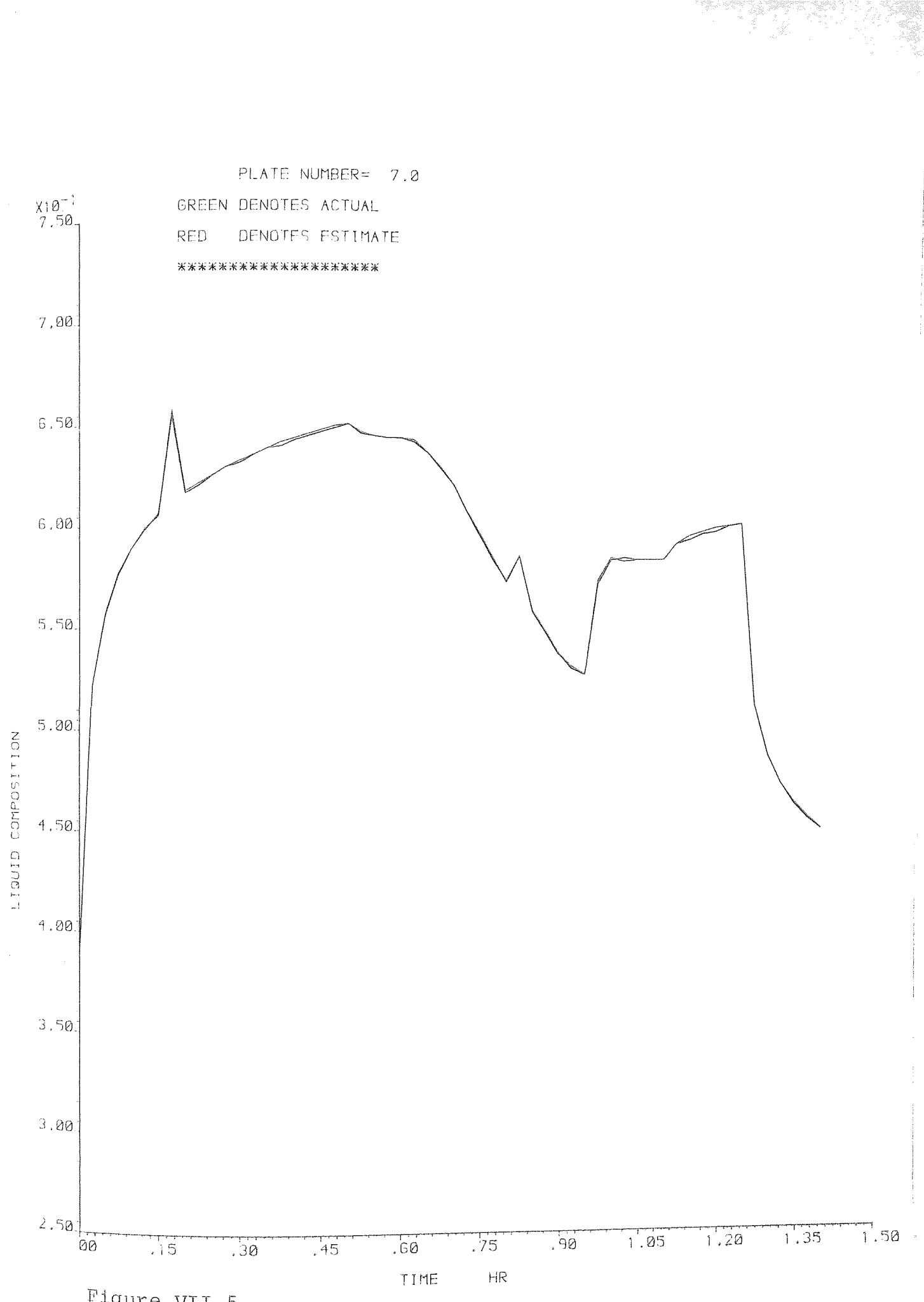


Figure VII.5
Simulated actual and estimated liquid compositions on the feed tray where a corrupt temperature measurement is taken

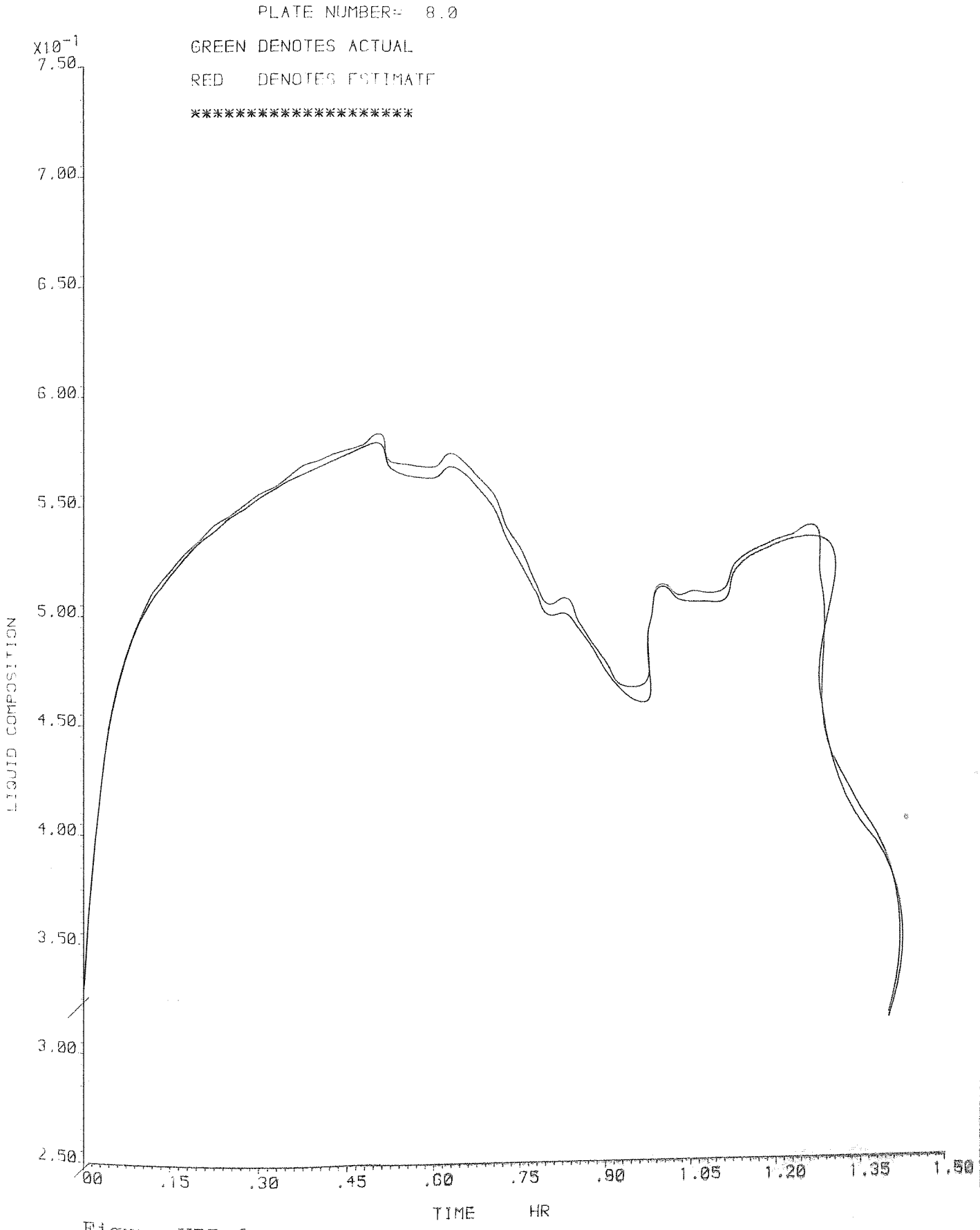


Figure VII.6
Simulated actual and estimated liquid compositions on a tray in the stripping section

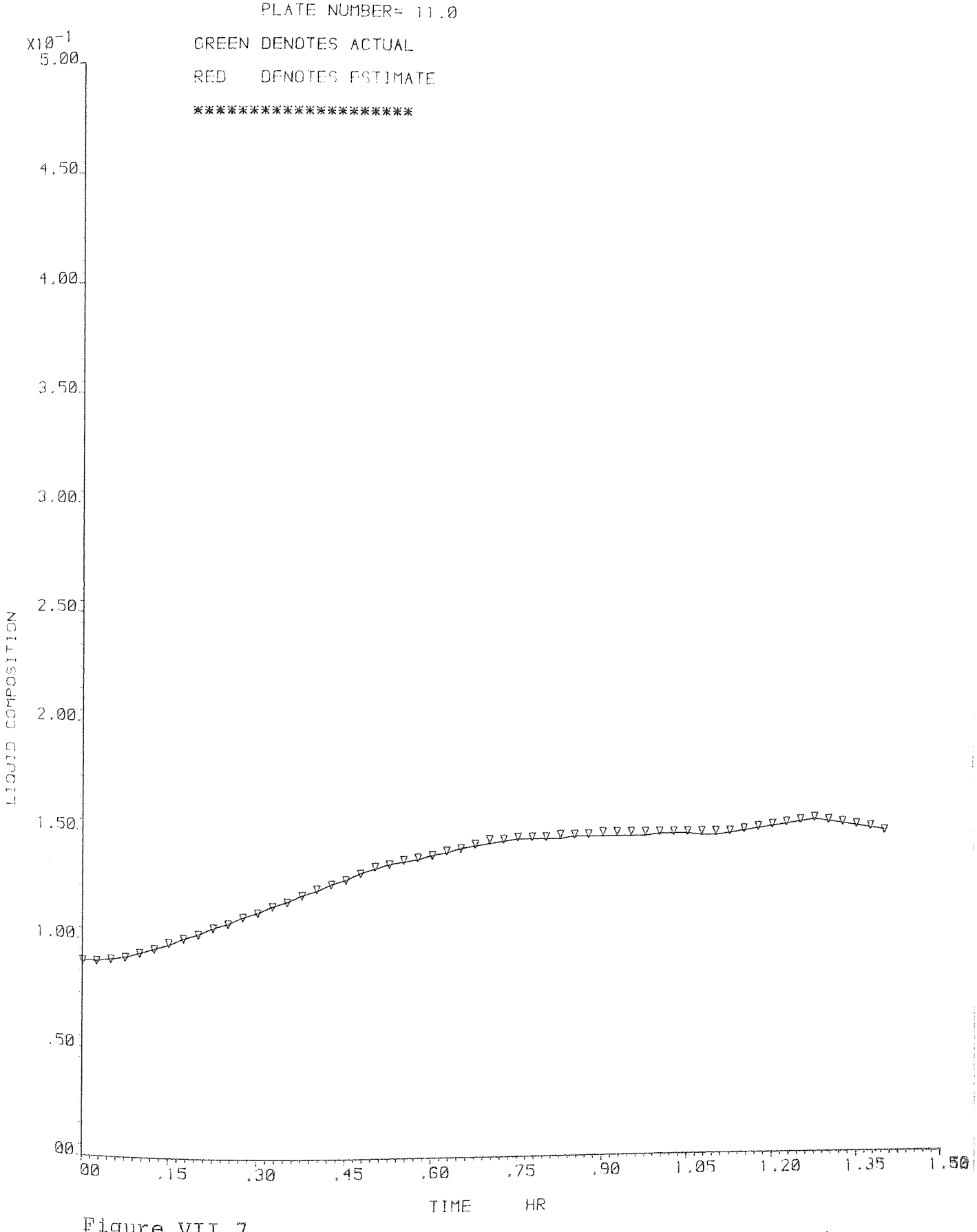


Figure VII.7
Simulated actual and estimated bottom product compositions

Figure VII.8
Simulated multiple step changes in feed rate which is supplied to the filter as a noisy measurement and the estimate produced by the filter. An example of the smoothing action of the filter in the face of intense measurement noise

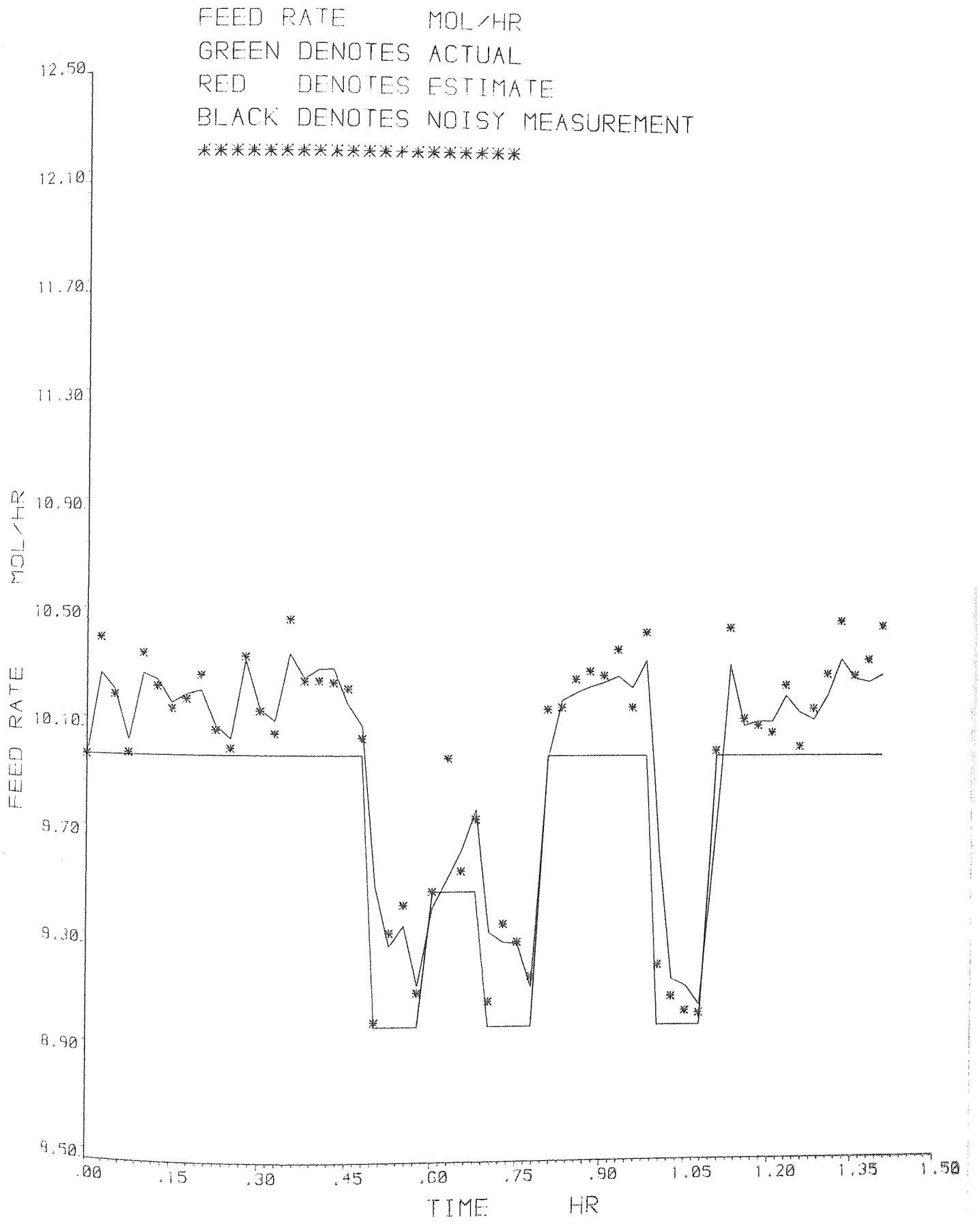
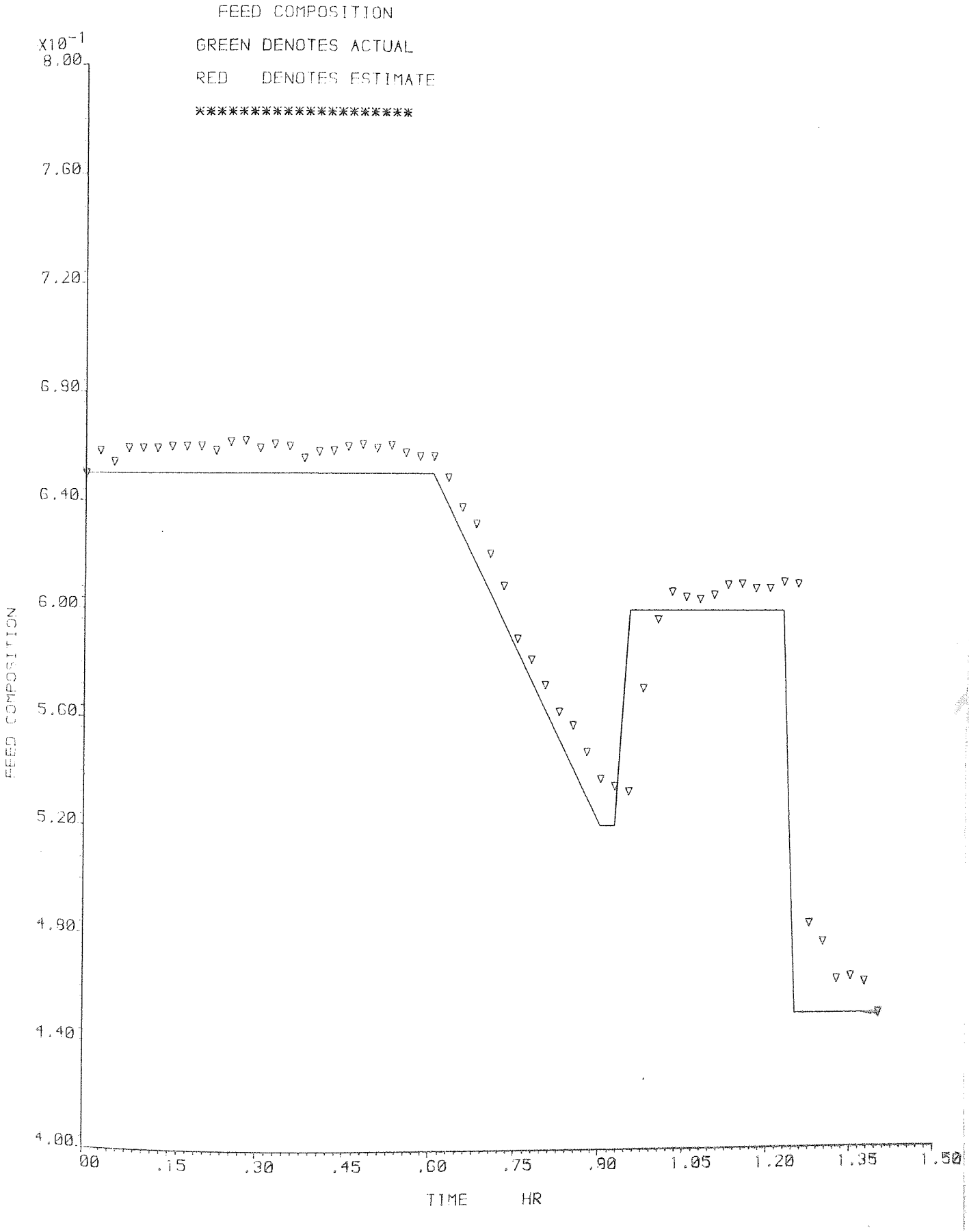


Figure VIII.
Simulated changes in the feed composition which is supplied to the filter as a parameter to be estimated and the estimates produced by the filter are compared



VIII.7 DISCUSSION OF THE SIMULATION RESULTS

Generally speaking, it appears that the proposed methodology for the extension of linear filtering theory to nonlinear systems is very effective in that it has almost eliminated the stability problems associated with estimation of a highly nonlinear system with highly nonlinear measurement functional relationships with sample times of up to 40 seconds.

Regarding the tuning of Kalman filters, it appears that this aspect of the design has been rather exaggerated in the past. Although, it may be somewhat lengthy, it certainly is not insurmountable given that the designer approaches the problem with inspired thought and a knowledge of the degree of inaccuracy of the filter's system model and the degree of uncertainty of the measurements. The absolute accuracy of the filter's system model is a secondary consideration. Within reason, no matter how inaccurate the predictions may be, the filter should be able to produce an estimate of the state of the system so long as the inaccuracies are reported to the filter through the Q matrix. Obviously the quality of the estimate may deteriorate if the filter model is highly inaccurate and in the extreme cases when the model is "too" inaccurate, the estimates may diverge gradually. This is consistent with the notion of seeking an "adequate" filter model (discussed in Chapter VI) that is neither too complex nor too inaccurate but

just delicately balanced. As regards this particular column, the simulation results in Chapter V indicated that the predictions of the filter model (Model I) can differ from the column simulator (Model II) by approximately 10% in terms of composition and in the order of 1% in terms of holdups. These values were good guidelines in starting the tuning procedure. Similar simulation studies can help in any tuning exercise.

With reference to this particular column, the simulation results (Figures VII.3 to VII.9) show that EKF3 is capable of estimating and tracking the tray liquid compositions very accurately from a handful of highly corrupted temperature and flow measurements. The more measurements available, the better the estimates. On this column, the temperature measurements in the stripping section are closer to each other than the enriching section (see Figure VII.2) and therefore the estimates are more accurate in the stripping section.

In Figures VII.3, VII.4 and VII.6 the displayed results are, in actuality, slightly distorted due to the fact that the plotter fits a curve to the points. Had the points been simply joined by straight lines, as in Figure VII.5, the estimates would have been almost indistinguishable from the actual values which is a good reflection of the accuracy of the estimates produced.

In Figure VII.8, the random noise has been added to the measurements as a positive noise which effectively appears as a bias and, if anything, should make life more difficult for the filter. However, this does not seem to trouble it in any way which is further proof for its robustness. Had the noise been added as a zero mean, the estimates would have been more accurate (see Appendix E).

The ability of EKF3 to estimate and track the unmeasured feed composition regardless of sub-cooling of the feed stream (Figure VII.9) should interest control practitioners especially the advocates of feedforward control. The average inaccuracy of the estimates was less 0.5% over 1.5 hours. It also appears that the filter prefers ramp changes to large step ones.

To sum up these results highlight the following powerful features of EKF3:

(i) its ability to function as a low-cost, fast and accurate on-line analyser with a sample time of only 18 seconds without the associated hardware problems inherent in the operation of on-line analysers. This result is quite encouraging in that it opens tremendous possibilities for overcoming hardware problems by the relatively inexpensive software approach

(ii) its advantages of accurately estimating the state from secondary measurements as an aid to control

cannot be over emphasized. This will be discussed further in Chapter VIII.

C H A P T E R E I G H T

ESTIMATOR-AIDED FEEDFORWARD COMPUTER CONTROL SIMULATION STUDIES

VIII.1 INTRODUCTION

In distillation control, it is generally acknowledged that composition control is superior to temperature control. However, on-line measurement of composition is expensive and the measurement lags and sampling delays associated with the measurement are so large as to make it difficult to design even an effective feedback control system. Therefore, the capability of the extended Kalman filter (EKF2 and EKF3) to function as an on-line analyser has already made it a potentially attractive aid to control considering that there are no appreciable time lags in the estimation of tray compositions. Hence, having come thus far, even with feedback composition controllers which use the estimated compositions as inputs, better control must already be within reach.

Feedback controllers, even when designed by the superior multivariable design methods, have not really proven themselves capable of providing optimum control for the slow-moving chemical engineering systems that are subject to unknown disturbances and one cannot help wondering if they ever will. The problems inherent in the stability aspects of these controllers make them even less attractive. Therefore, in this research it is chosen to move away from the feedback control philosophy as far as possible.

VIII.2 ESTIMATOR-AIDED FEEDFORWARD CONTROL

Since the extended Kalman filter (EKF3) is capable of estimating the known and unknown input disturbances as they enter the system (e.g. feed rate and composition in binary distillation), it becomes very desirable for integration into a feedforward (predictive) control algorithm as shown in Figure VIII.1. Having refined the state and parameters of the system at time t, the state can then be integrated forward to the next sample time, $t+\delta t$, at computer speed to predict the deviations in the controlled states. The predicted deviations can then be fed into the controller which, in turn, computes the control signals required and outputs them to the plant.

Implicit in this picture, also, is the role of the computer which performs the calculations inherent in estimation and also functions as the data acquisitioner and controller.

It now remains to consider the controller synthesis aspects of this proposal. In a single conventional PI controller, by synthesis it is simply meant that the values of K and τ_I need to be determined. Obviously, for complex multivariable systems, one would resort to the multivariable design methods. The multivariable design methods are almost invariably based on linear control theory and thus require that the nonlinear system model be linearized about a

nominal state. Computers can now enable us to consider piecewise linearization and thus synthesis at every sample time to provide better and more stable control. This means that one is effectively proposing a totally adaptive feedforward control structure in which the system model and its controllers can be adapted to the system as time proceeds.

VIII.3 THE CONSTRAINTS IMPOSED BY THE INTERSAMPLE CALCULATION LOAD

The major ostensible drawback of this proposal may stem from the fact that in on-line real time applications, a considerable amount of calculations may have to be performed during the sample time - especially in high dimensionality systems. In order to construct a stable extended Kalman filter the sample time must be less than one minute in highly nonlinear systems with highly nonlinear functional measurement relationships. This, at first sight, may appear to be a daunting prospect. But it need not be. The truth is that microprocessors (141) have already offered a plausible solution to this problem. If the intersample computation load is excessive, it can be delegated to a number of microprocessors which are supervised by a minicomputer. This means that one is speaking of a parallel-processor arrangement in which the independent parts of the intersample calculations take place simultaneously to save time.

Although microprocessors can help alleviate this problem, an excessive amount of intersample calculation is never desirable. Thus attempts must be made to reduce it where and whenever possible. As regards the construction of the estimator, the model reduction aspects of the design become even more important. An adequate low order filter model, can greatly cut the calculations involved in the estimation part of

this control method. Also, redesigning the controllers at every sample may not be totally justifiable. It may be that controller parameters are best treated as pseudo state variables and estimated stochastically. Such considerations must never be foregone.

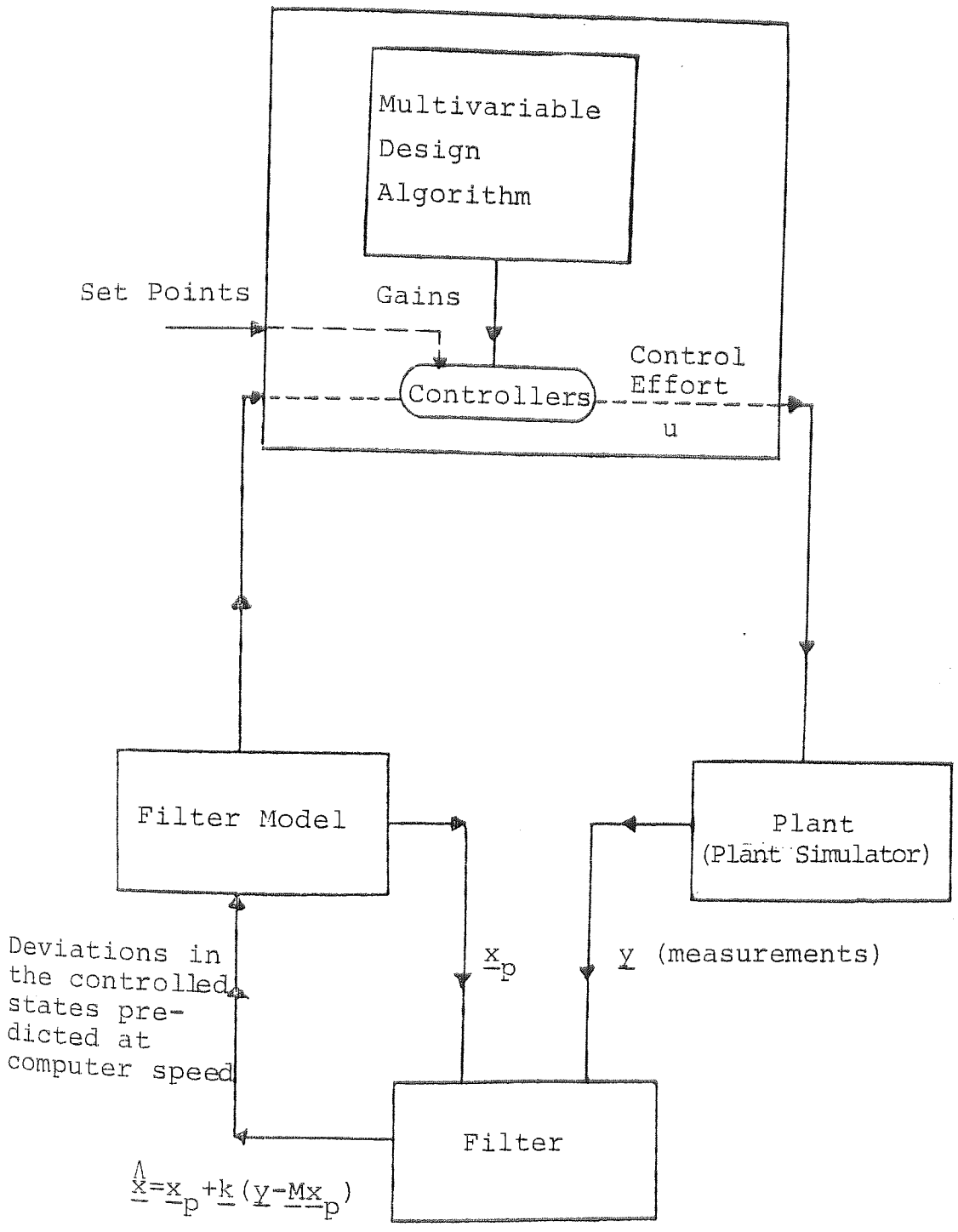


FIGURE VIII.1 - Implementation of Estimator-Aided Feedforward Computer Control

VIII.4 THE CHOICE OF MEASURED AND MANIPULATED VARIABLES

So far, the discussion has presupposed an available control configuration in that we have assumed that the measured and manipulated variables (or control inputs) have already been selected and interconnected. A control configuration is normally characterised by:

(i) a set of variables which are to be controlled to achieve a specified objective

(ii) a set of variables which are to be measured for control purposes

(iii) a set of manipulated variables

(iv) a certain structure for interconnecting the measured and manipulated variables

The first class of control objectives (e.g. product quality control) dictates directly the measurements which should be made for monitoring the process. These primary theoretically desirable measurements are not always available. Often they have to be substituted by secondary ones. This is where the filter plays an important role. The choice and number of secondary measurements and their associated estimation problems can be examined independently of other decisions. THe following factors can affect the choice and the number of the secondary measurements:

(i) economic factors

(ii) engineering judgement

(iii) theoretical considerations such as observability criterion for the estimator

Selection of the manipulated variables will affect the response capability to external disturbances and the ability to keep the controlled states at their desired values continually. The more manipulated variables available, the better will be the control of the process. Almost invariably, structural aspects of the processing systems and the physicochemical equations describing the processing unit are the dominant factors in establishing feasible sets of manipulated variables. Govind and Powers (141) have listed a number of qualitative conditions that the selected manipulated variables should satisfy. Among these are reliability, ease of operation, startup and shutdown, and to avoid the manipulation of variables which influence a large number of other variables.

It now remains to consider the interconnection of the measured and manipulated variables. Solution to this will again be guided partly by engineering judgement and partly by theoretical considerations. Engineering judgement usually draws on the past experience and is more relevant to simple systems while methods such as degrees of freedom studies or modal analysis can provide a powerful basis for the theoretical approach for complex processes such as

distillation.

The final stage of the exercise is the synthesis of the controllers. It is almost universally recommended that multivariable design methods should be used for multivariable processes. Such methods include:

(i) multivariable feedforward

(ii) optimal feedforward

VIII.5 THE MAIN FEATURE OF ESTIMATOR-AIDED FEEDFORWARD (EAFF) CONTROL

For convenience of notation, estimator-aided feedforward control will henceforth be abbreviated to EAFF control. EAFF control is essentially characterised by:

(i) its feedforward philosophy which largely minimises the undesirable effect of time lags on the system's response. Also, EAFF controllers do not appear to suffer from the stability problems which can arise during the simultaneous operation of feedback controllers

(ii) a number of controllers preferably designed by the multivariable design methods

(iii) nonlinear dynamics and linear or piecewise linear control

(iv) feedback information through the estimator which promotes self-correction

(v) its adaptive nature in that the model can be made to track the system, its parameters, and its controller parameters

VIII.6 APPLICATION OF EAFF CONTROL TO BINARY DISTILLATION

The distillation column discussed in Chapter III is used as an example. The binary liquid system is trichloroethylene (MVC) and tetrachloroethylene mixture with the composition of MVC in the feed equal to 0.65.

VIII.6.1 THE CONTROL OBJECTIVE

The objective is to control the liquid compositions on trays 1 and 10 at their desired setpoints regardless of the known and unknown disturbances introduced randomly or deterministically.

VIII.6.2 THE MANIPULATED VARIABLES

The possible manipulated variables are:

(i) the distillate offtake rate

(ii) the bottoms offtake rate

(iii) the heat input rate

(iv) the reflux rate

Of these the distillate and bottoms offtake rates are needed to control the reboiler and reflux drum holdups to get the column to operate under steady-state conditions. Therefore, the heat input and reflux rates are available for composition control.

The counterpart of this configuration in the feedback temperature-control sense is to use the temperature on tray 1 to control the reflux rate and the temperature on tray 10 to control the heat input rate (Figure VIII.2). The performance of EAFF control will be compared with this control structure quantitatively. The performance index will be the familiar Integrated Absolute Error (IAE) criterion:

$$IAE = \int_{T_1}^{T_2} \{ |(x_1 - x_{1,s})| + |(x_{10} - x_{10,s})| \} dt$$

where

x_j and $x_{j,s}$ are the liquid composition on the jth tray and its desired setpoint

and here T_2 is chosen to be T_1+55 minutes

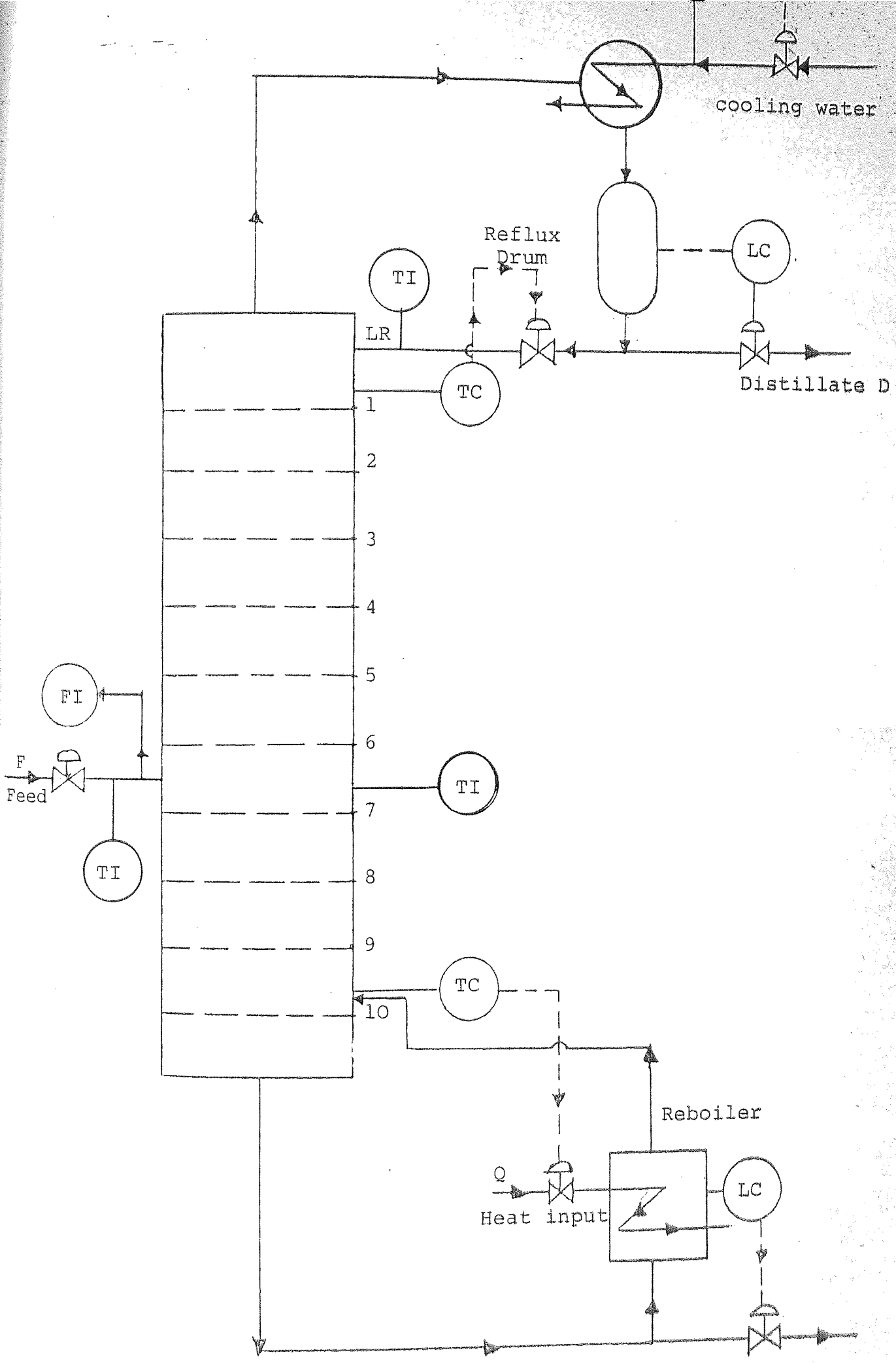


FIGURE VIII.2 - The Feedback Temperature Control Scheme used for Comparison with EAFF Control

VIII.7 CONTROLLER DESIGN

VIII.7.1 EAFF SCHEME

As the starting point two PI controllers are used in the EAFF control scheme. These controllers were designed individually by the reaction curve method (1) on the column simulator. They were then detuned to allow for interaction when operating simultaneously.

The method of implementation of these controllers on a digital computer is discussed by Daie (134). The controller equations are

$$LR = LR_s - 100.0\left(e_{t,i} + \frac{1}{0.009}\sum_{i=1}^{n} e_{bi}\right)$$

$$Q = Q_s + 800.0\left(e_{b,i} + \frac{1}{0.0018}\sum_{i=1}^{n} e_{b,i}\right)$$

where

$e_t = x_1 - x_{1,s}$

$e_b = x_{10} - x_{10,s}$

LR = reflux rate mol./hr.

Q = heat input kJ./hr.

LR_s and Q_s the steady-state biases for R and Q respectively

$x_{i,s}$ are the setpoints

The two PI temperature controllers used were also designed using the reaction curve method and detuning on the column simulator. The controller equations are:

$$LR = LR_s + 150\left(e_{t,i} + \frac{1}{0.015}\sum_{i=1}^{n} e_{t,i}\right)$$

$$Q = Q_s - 30.\left(e_{b,i} + \frac{1}{0.0027}\sum_{i=1}^{n} e_{b,i}\right)$$

where

$$e_{t,i} = T_1 - T_{1,s}$$

$$e_{b,i} = T_{10} - T_{10,s}$$

and $T_{i,s}$ are the temperature setpoints

VIII.8 EAFF CONTROL SIMULATION PACKAGE : THE MAIN PROGRAM SEGMENTS

The main program segments for EAFF control simulation are essentially the same as those in the estimation package except that two more subroutines are added. These are:

SUBROUTINE CONSET - Subroutine to define the controller settings

SUBROUTINE CONTR2 - Subroutine to implement two PI controllers

The main program arrangement is shown in Figure VIII.3. THe full documentation of this package is given in Appendix F (Microfiche).

VIII.9 FEEDBACK TEMPERATURE CONTROL SIMULATION PACKAGE

This package is obtained simply by inserting a subroutine in the process simulator to implement two PI feedback temperature controllers. The main program arrangement is depicted in Figure VIII.4.

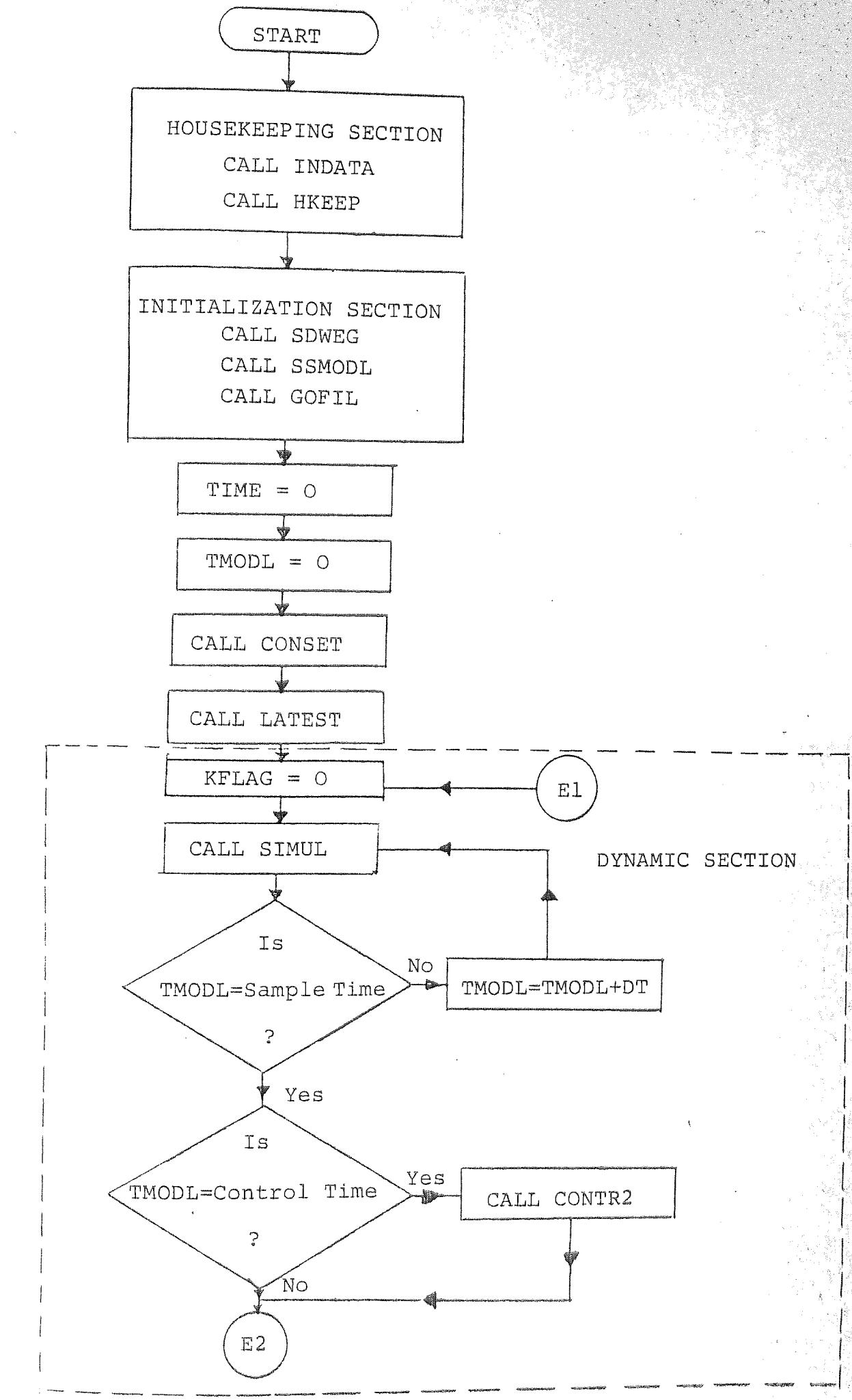


FIGURE VIII.3 - The Main Program Arrangement for EAFF Control Package

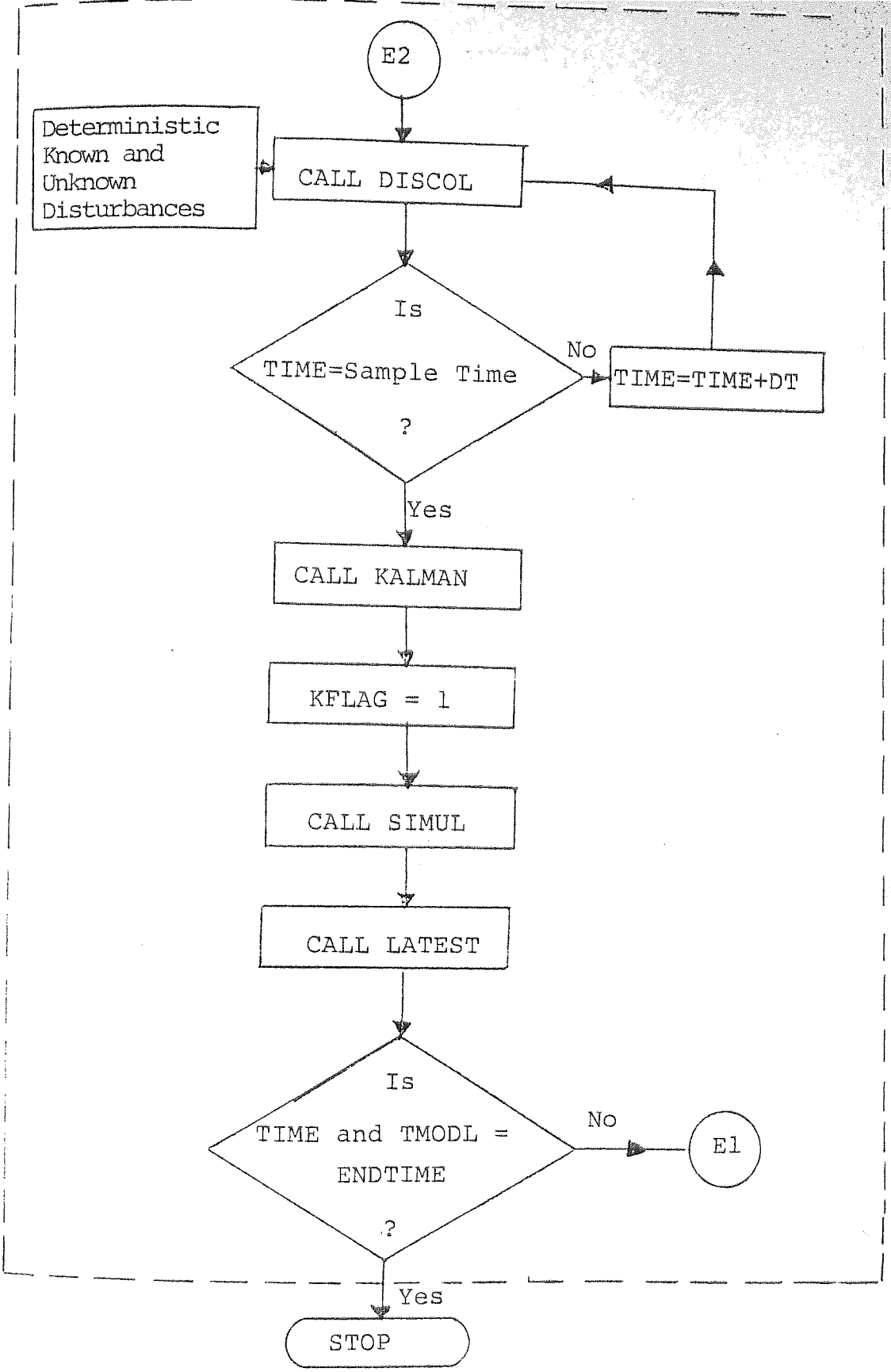


Figure VIII.3 Continued

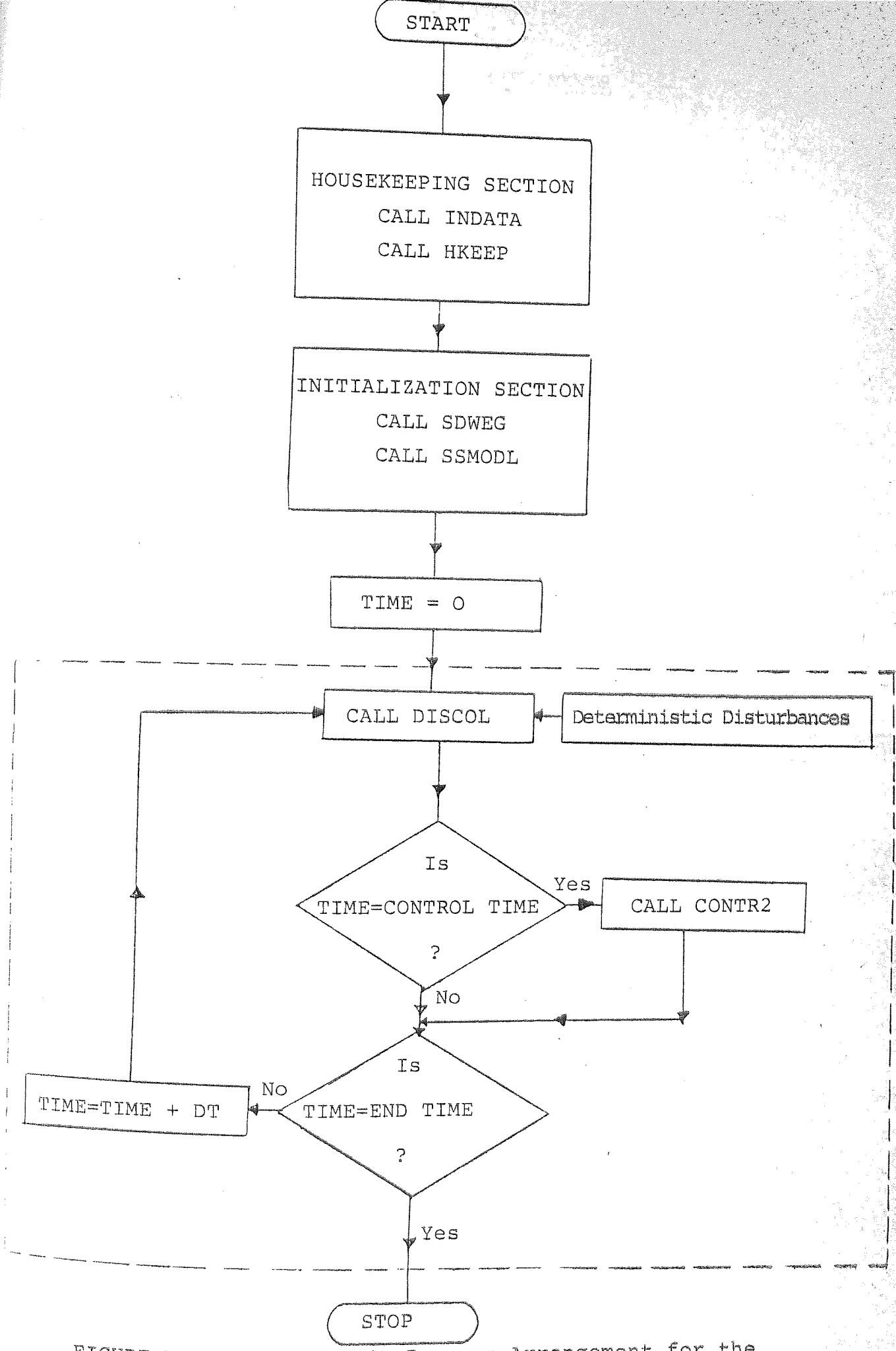


FIGURE VIII.4 - The Main Program Arrangement for the Implementation of Feedback Temperature Control

VIII.10 CONTROL SIMULATION EXPERIMENTS

The following experiments were carried out to assess and demonstrate the advantages offered by EAFF control and its promising features:

(i) the response of the column to a 10% sustained step increase in the feed rate under EAFF control compared with its response under feedback temperature control. The responses are compared graphically (Figures VIII.5 and VIII.6) and quantitatively via their respective IAE's. The sample time was chosen to be 18 seconds. The IAE's were found to be

EAFF control : IAE ≈ 0.004 over 55 minutes

feedback temperature control : IAE ≈ 0.008 over 55 minutes

(ii) introducing multiple disturbances in the feed rate, composition and temperature and comparing the responses of the column under the two control schemes, i.e. EAFF control and feedback temperature control (see Figures VIII.9 and VIII.10). The sample time was 18 seconds

(iii) increasing the sample time to 25 seconds with the same multiple disturbances as in experiment 2. The EAFF controllers were still stable and no further tuning was necessary. However, as expected, the overall performance did suffer slightly compared with the case with a sample

time of 18 seconds. This result is produced digitally in Appendix F (Microfiche)

(iv) The sample time was reduced to 10 seconds with the same disturbance as in experiments 2 and 3. EAFF control produced almost perfect results in that the transients in the controlled variables were hardly conspicuous

VIII.11 REMARKS ON THE DISPLAYED CONTROL SIMULATION RESULTS

Figures VIII.5 and VIII.6

The responses of the column to a 10% sustained step increase in the feed rate under EAFF and feedback temperature controllers are compared. The sampling interval for the EAFF control was chosen to be 18 seconds - well within the dominant time constant of the system. It can be seen that the controlled variables undergo less transients under EAFF control and take less time to return to their respective setpoints. The feedback temperature controllers are very tightly tuned and, therefore, the computed IAE of 0.008 associated with them is very conservative. In real-life one would not risk tuning the controllers so tightly and thus the IAE would be greater than 0.008 which is further proof for the superiority of EAFF control whose IAE was approximately 0.004 over the same time interval. It is also worth noting that these results are obtained on a column with a reboiler whose manipulated variable contains minimal time lag. On a larger column and in the face of a time lag in the manipulated variable's response, the performance of the feedback controllers would be expected to deteriorate markedly whereas the EAFF controllers should not be troubled by these

problems by the virtue of their feedforward philosophy.

Figures VIII.7 and VIII.8

These graphs highlight the second interesting difference between the feedback temperature and EAFF controllers. It can be seen that EAFF controllers find the new values for the manipulated variables for the new steady-state more rapidly. Naturally, this is an additional advantage in that it means much less off-specification tray compositions are produced in the face of a sustained step increase in the feed rate.

Figures VIII.9 and VIII.10

The response of the column to multiple disturbances in the feed rate, composition and temperature under EAFF and feedback temperature controllers are compared. It can be seen that regardless of the type and time of the disturbances the EAFF controllers restore the controlled variables to their setpoints efficiently. Although, under feedback temperature controllers, the controlled variables appear to tend towards their setpoints initially, as further disturbances are introduced they become oscillatory indicating that the column is tending towards instability. This is a good example of the

robustness of the EAFF controllers in that they continue to perform well without any need for further tuning.

Figures VIII.11 and VIII.12

Another demonstration of the orderly manner in which the control inputs are manipulated to restore the controlled variables to their desired setpoints by EAFF controllers. Notice that in Figure VIII.11, the boilup rate is plotted against time instead of the actual heat input rate, Q. The variations of the boilup rate should portray the variations in Q. Thus EAFF control appears to be more economical in terms of energy consumption too.

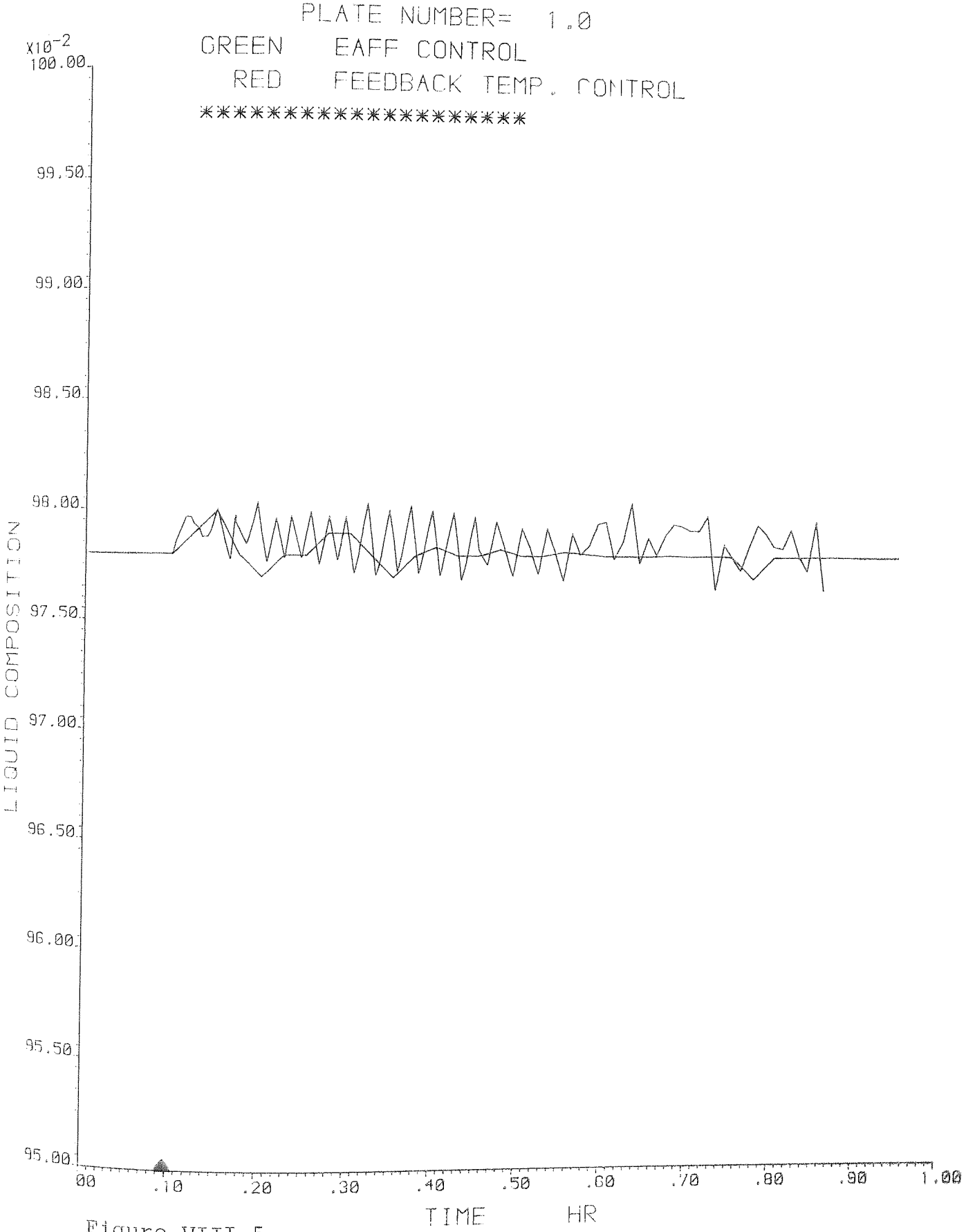


Figure VIII.5
The responses of the column to a 10% step increase in the feed rate under EAFF control and feedback temperature control

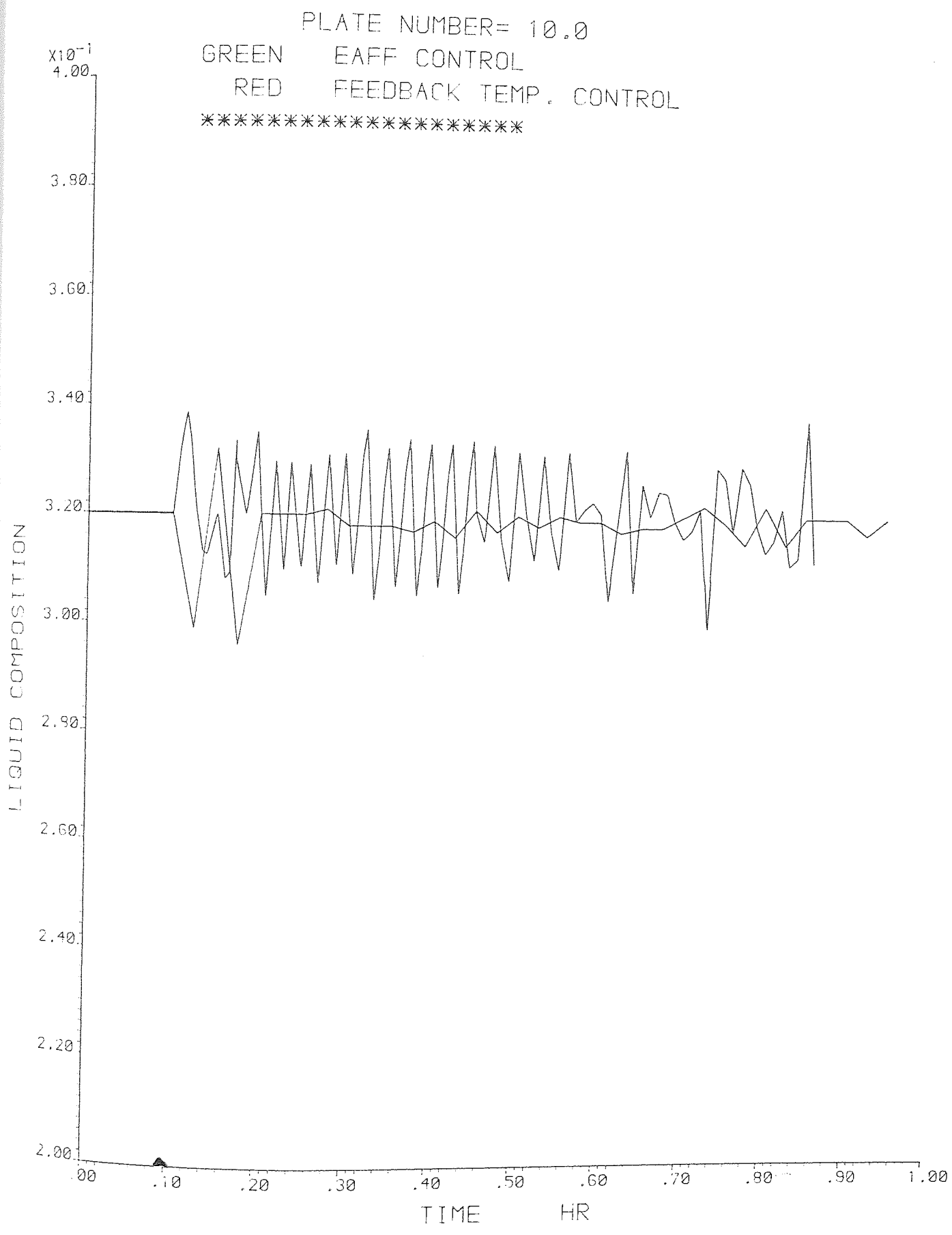
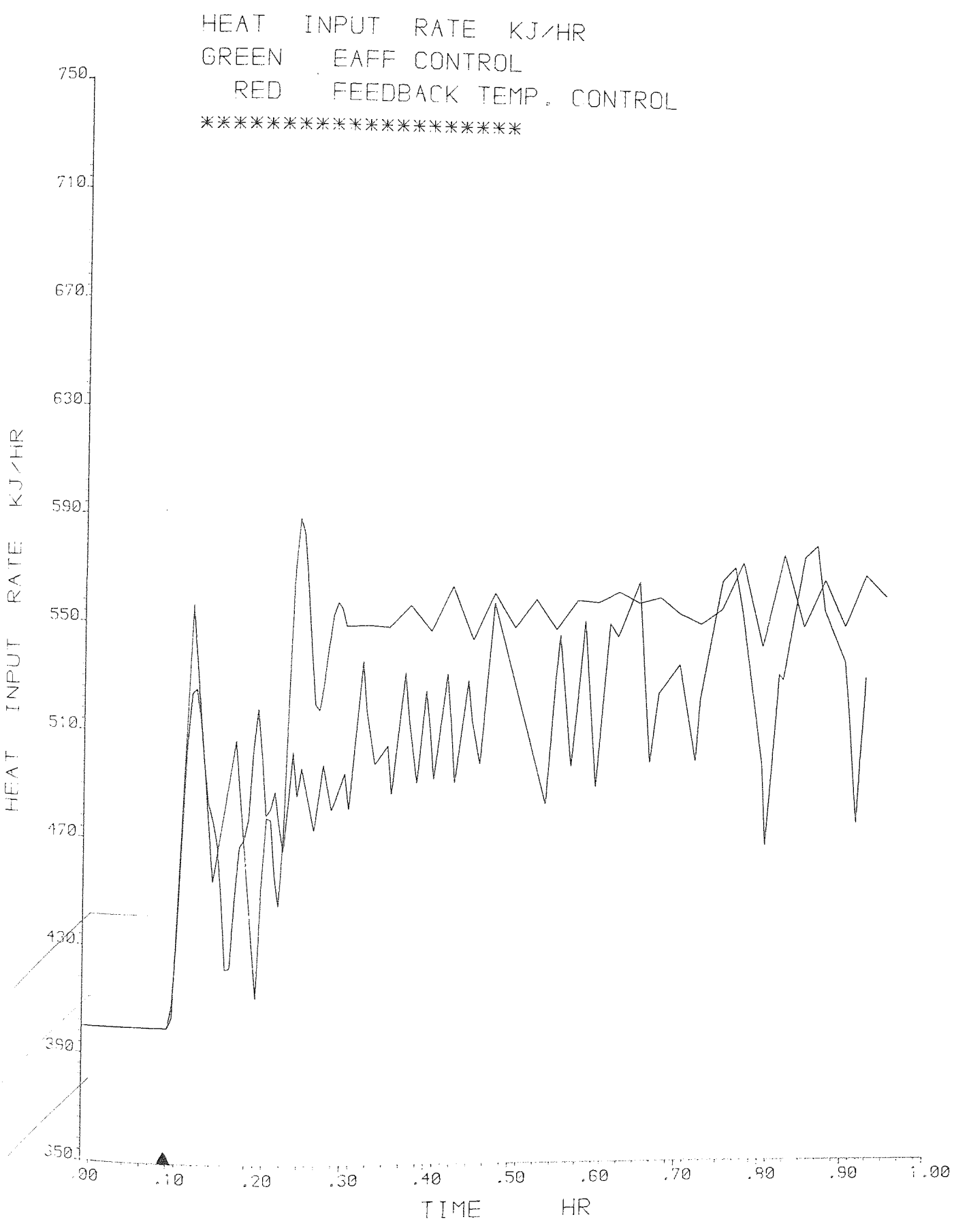


Figure VIII.6
The responses of the column to a 10% step increase in the feed rate under EAFF control and feedback temperature control

Figure VIII.7
Manipulation of the heat input rate by EAFF controllers compared with the manipulation by feedback temperature controllers when the column is subjected to a 10% step increase in the feed rate



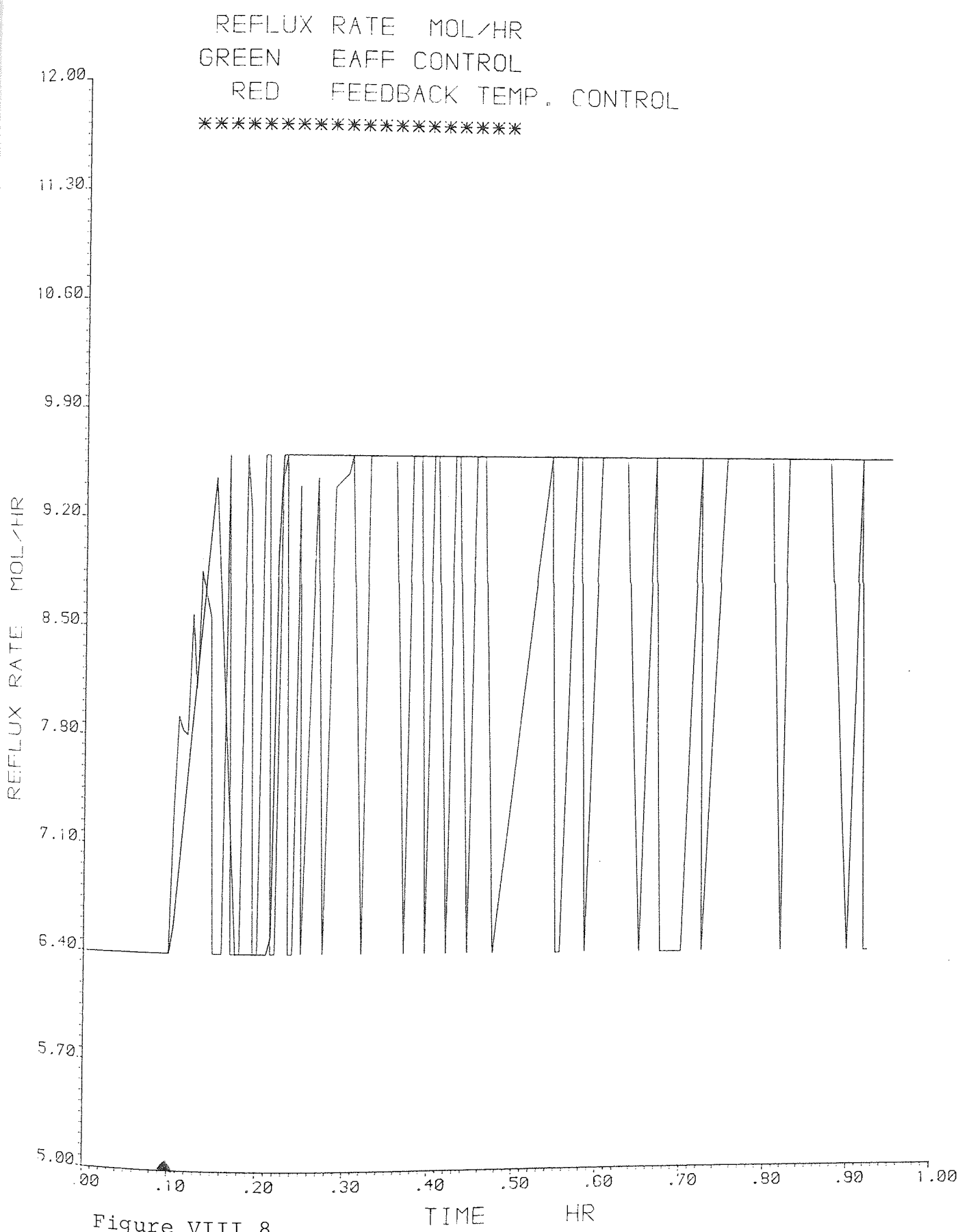


Figure VIII.8
Manipulation of the reflux rate by EAFF controllers compared with the manipulation by feedback temperature controllers when the column is subjected to a 10% step increase in the feed rate

Figure VIII.9

The responses of the column to multiple changes in the feed rate, composition and temperature under EAFF control and feedback temperature control

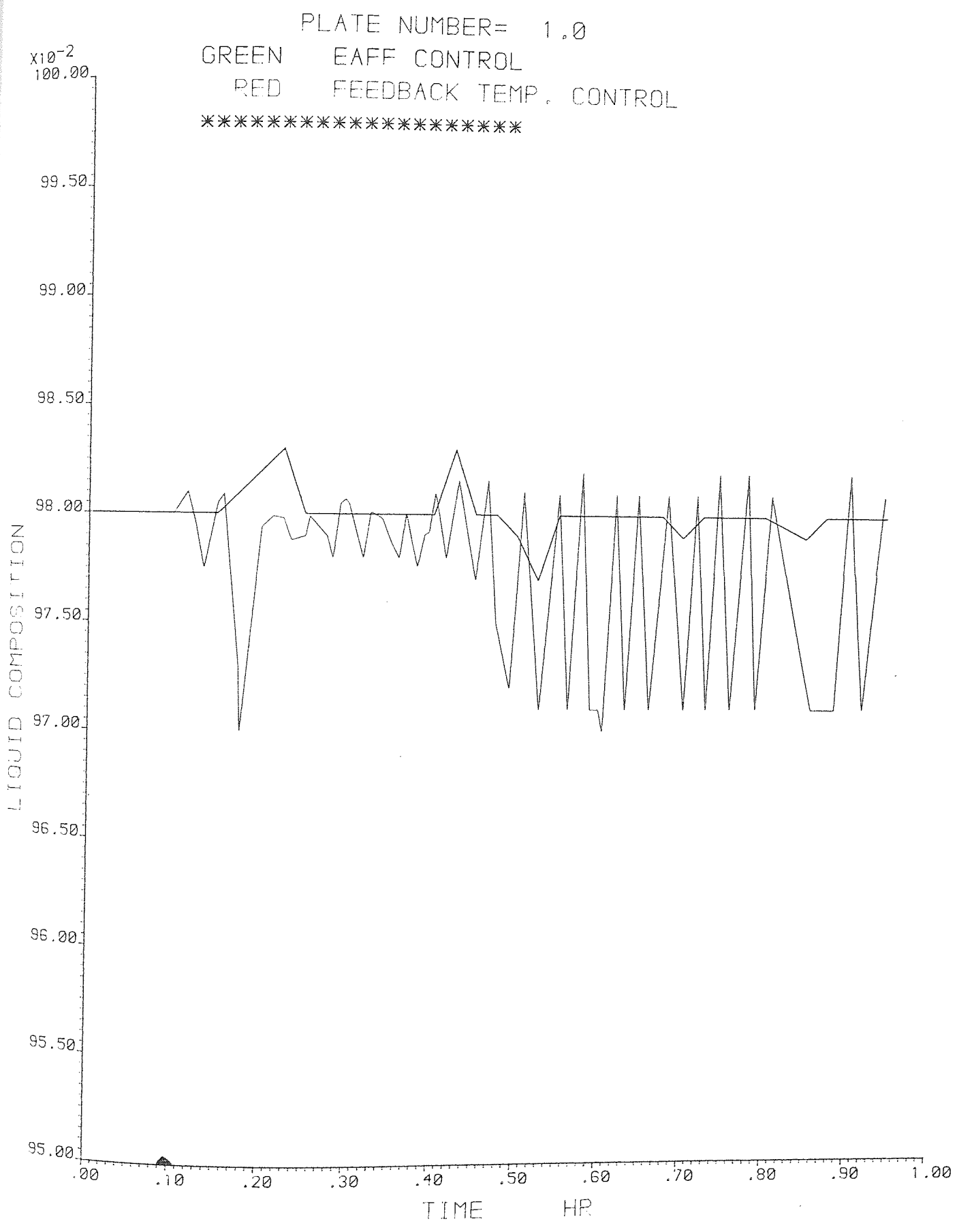


Figure VIII.10

The responses of the column to multiple changes in the feed rate, composition and temperature under EAFF control and feedback temperature control

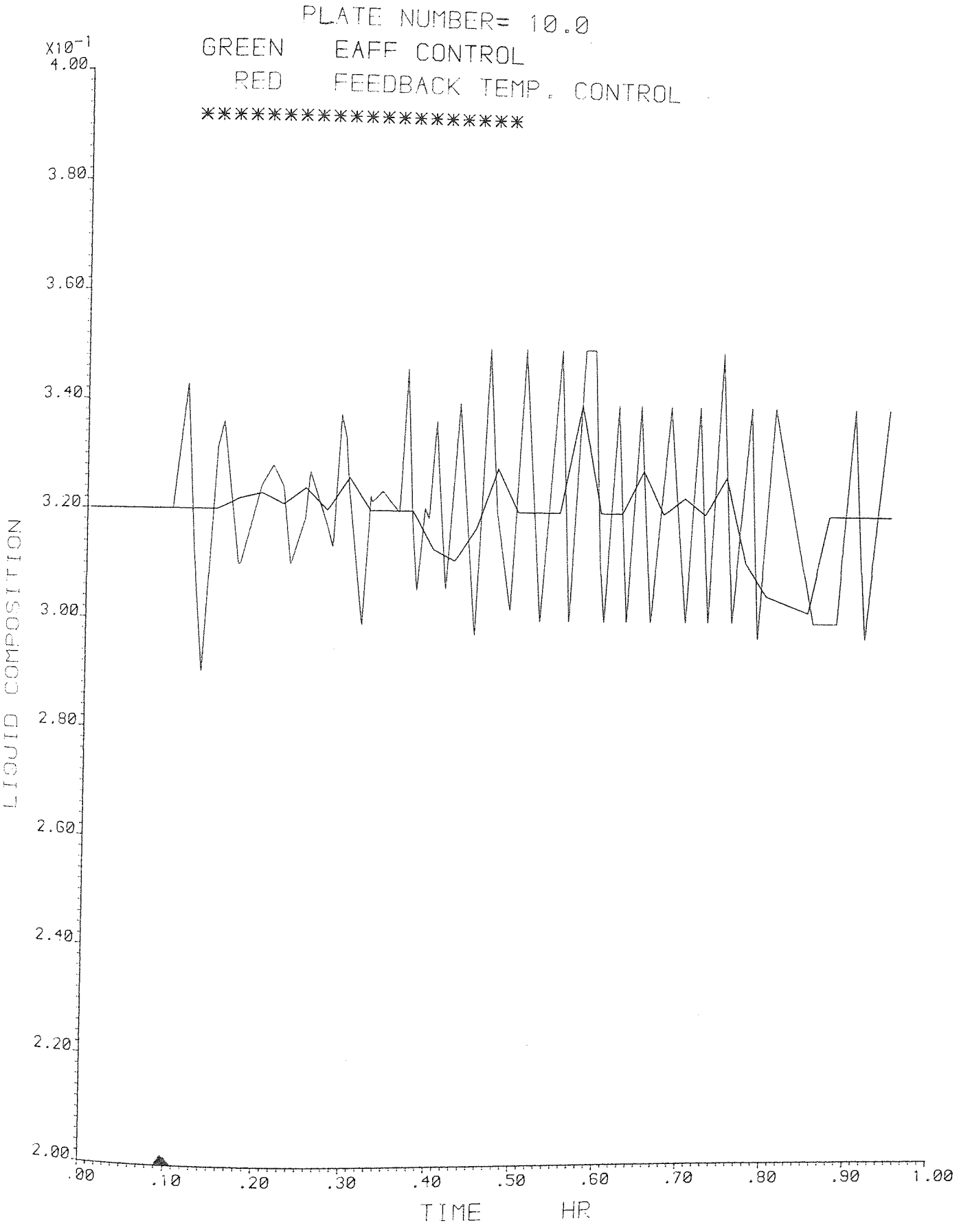


Figure VIII.11

Manipulation of the boilup rate by EAFF controllers compared with the manipulation by the feedback temperature controllers when the column is subjected to multiple changes in feed rate, composition and temperature

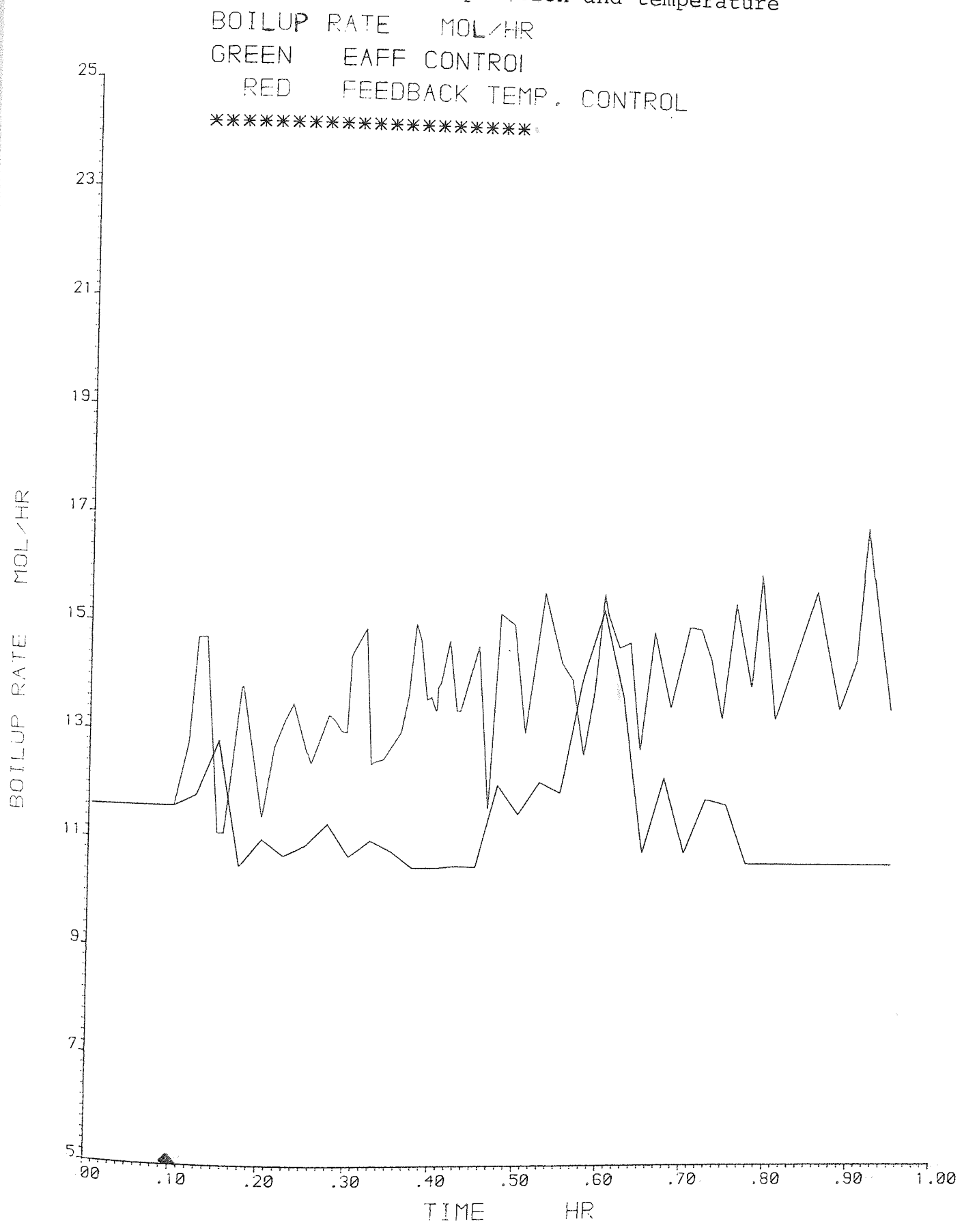
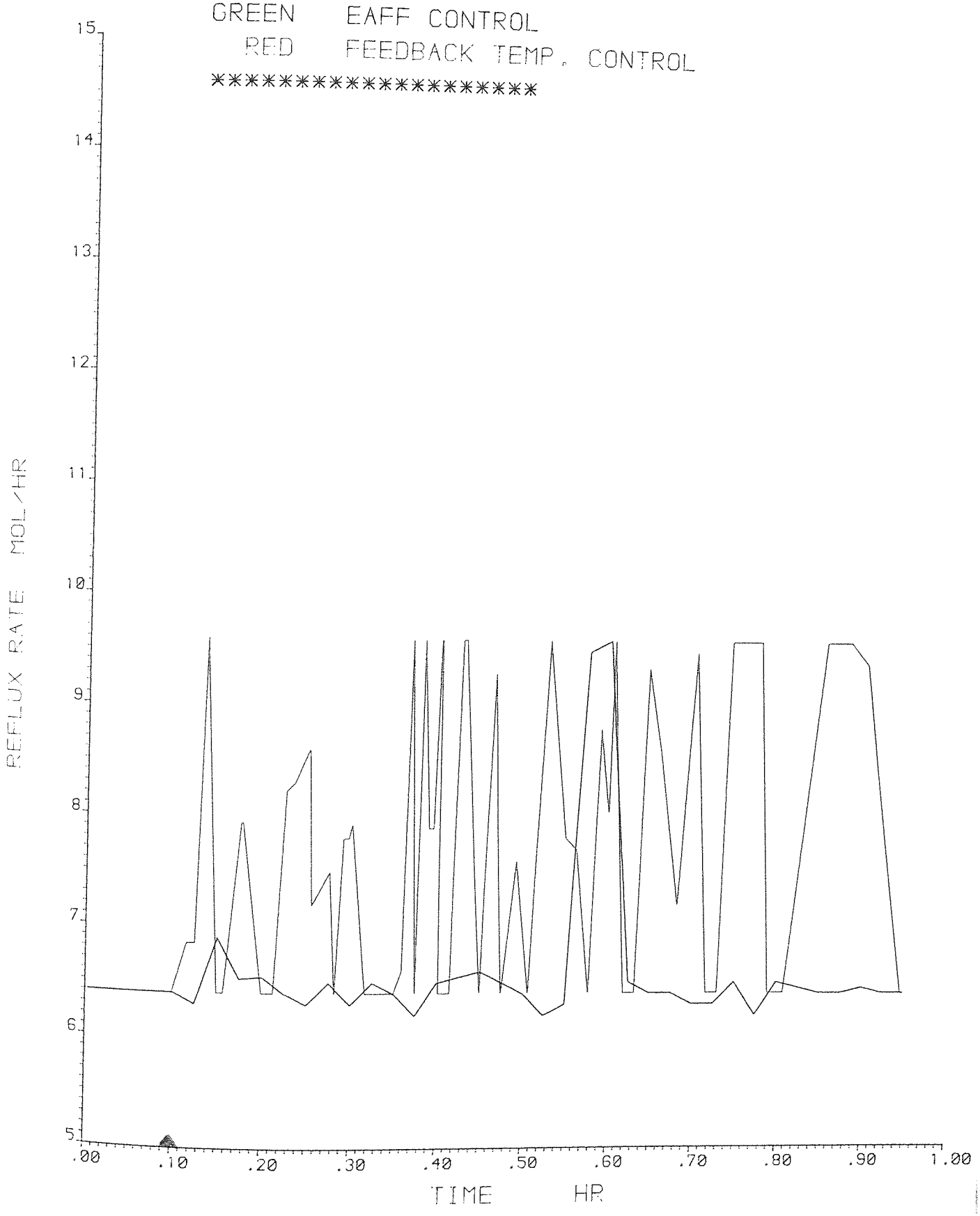


Figure VIII.12

Manipulation of the reflux rate by EAFF controllers compared with the manipulation by feedback temperature controllers when the column is subjected to multiple changes in feed rate, composition and temperature



VIII.12 DISCUSSION OF CONTROL SIMULATION RESULTS

From Figure VIII.5 and VIII.6 it can be seen that EAFF controllers take much less time to settle and bring the compositions to their desired values than the feedback controllers. These graphs also highlight the typical interaction effects that occur during the operation of multiple feedback controllers whereas the EAFF ones do not appear to suffer from these problems.

Even on a column wih a reboiler whose manipulated variable contains minimal time lag, the performance of EAFF controllers is still twice as good as the feedback ones in terms of their respective IAE's. One of the main advantages of EAFF control lies in its ability to combat the undesirable effect of time lags on the system's response whereas the performance of feedback control would be expected to deteriorate dramatically in the face of time lags. Therefore, comparatively speaking, in a more realistic situation and on a larger column, EAFF control should be even more effective and robust than feedback.

Another interesting feature of EAFF control is that it appears to be capable of finding the right adjustments to the manipulated variables much more efficiently (see Figure VIII.7 and VIII.8). This is advantageous in terms of the economy of operation in that it means less off specification tray compositions. EAFF control also appears to be more economical in

terms of energy consumpsions (see Figures VIII.11). This is the second most attractive feature of EAFF control.

The sampling interval chosen for EAFF control during this experiment was 18 seconds - well within the dominant time constant of the column (20 minutes approximately). In an on-line real-time application another important consideration in choosing the sampling interval would be for it not to be too small so as to commit the control computer to just sampling the process instruments and not having time to perform other tasks.

When multiple disturbances were introduced into the column, the feedback controllers made the system unstable (Figures VIII.9 and VIII.10) which proves that in the previous experiment these controllers must have been very tightly tuned. Since in real-life one would not run the risk of tuning the controllers so tightly the computed IAE used for comparison with EAFF control is very conservative and this provides further proof for the superiority of EAFF controllers.

When the sample time was increased to 25 seconds, the EAFF controllers did suffer slightly and took a little longer to bring the controlled variables back to their desired values. This is because the same predictions of the state are used for estimation and for control. The bigger the sample time, the less accurate the predictions and the less accurate the

control. If, however, having computed the predicted state for control the filter model is reintegrated with the new values of the manipulated variables for estimation, the estimation and control should improve.

C H A P T E R N I N E

DISCUSSION AND RECOMMENDATIONS FOR FURTHER WORK

IX.1 DISCUSSION

The discussion of this research will include:

(i) the construction and instrumentation of the column

(ii) dynamic simulation

(iii) estimation

(iv) control

IX.2 THE CONSTRUCTION OF THE COLUMN

The original design and the present construction of the column deserve some discussion with reference to:

(i) the reboiler

(ii) the gravity flow arrangement

The reboiler is physically oversized which means that its holdup is disproportionately larger than that of a typical tray - by a factor of ten thousand. This makes the bottom product composition almost insensitive to load variations in the column and, therefore, pointless control. It was also found to be somewhat electrically under-powered as, even at the maximum setting, it just produced enough vapour to run the column at steady state and study its dynamics subject to throughput changes.

Due to financial constraints, the notion of gravity flow had to be employed in the reflux and

distillate lines by adding a pipe section to the top of the column. This arrangement was suspected to be problematical and this suspicion was later confirmed by the amount of trouble experienced during the operation of the column and also during the modelling of the heat losses from it. The main criticisms of this arrangement are:

(i) it makes the off-line modelling very difficult and the on-line modelling virtually impossible

(ii) it complicates the flow measurements unduly

(iii) it creates extra unwanted heat load for the reboiler

The problem of extra heat load on the already under-powered reboiler effectively hampered control experiments even with simple feedback temperature controllers.

For on-line estimation and control experiments the following modifications to the column are thought to be imperative:

(i) the notion of gravity flow must be abandoned and the associated pipe section should be removed. This will eliminate the extra heat load on the reboiler and may enable it to provide the extra heat needed for control experiments

(ii) the excessive reboiler holdup swamps the variations in the bottoms composition and thus makes it pointless to control the bottom

composition. A redesign of the reboiler is recommended - preferably one that contains a time lag in its manipulated variable's response in order to make it more comparable with an industrial column

It was decided to use a highly corrosive liquid system to ensure the robustness of the column. However, long-term exposure to the fumes from this liquid system can be hazardous and it is therefore recommended that it should be changed.

IX.2.1 THE COLUMN INSTRUMENTATION

The temperature and level measurements on the column are sufficiently accurate. However, the flow measurements need to be improved for on-line estimation and control. At least two accurate flow measurements are needed in the reflux and feed lines for on-line modelling. A more accurate level measurement at the reboiler may also be subservient to on-line modelling.

IX.3 DYNAMIC SIMULATION

The proposed structure for process simulators (Chapter IV) has proved to be flexible and computationally more efficient than the structures proposed for system simulation. It enables estimation and control routines to be simply inserted into the simulator with ease and little extra programming effort. The extensive simulation work carried out in this research was greatly facilitated by the flexibility of this structure.

As regards dynamic simulation of binary distillation using deterministic models the following points deserve some elaboration:

(i) the use of the AIChE tray efficiency calculation method

(ii) the use of Brambilla's equation to incorporate fluid dynamics into the models in the form of tray holdup calculation

(iii) the assumption of quasi steady state model for vapour rate calculation

The calculation of tray efficiencies by the AIChE method is worthwhile in that it enhances the accuracy of the static and dynamic simulations of distillation. The efficiencies are practically time-invariant during the transient periods for the type of disturbances that are likely to occur. However, during the simulation, they can be recomputed at a predetermined

frequency.

Brambilla's equation for tray holdup appears to be applicable to small diameter columns. In the truncated form of the equation used in this research, the A and B constants were determined from one set of experimental data and checked by subsequent experiments. The typical values provided by Brambilla (110) can serve as starting values during the determination of these constants for a particular type of column.

The stiffness implicit in the distillation models usually forces a small integration step size on their solutions. Hence to avoid excessive running times the policy should be to approximate differential equations by their steady-state counterparts as far as possible if the resulting inaccuracy is tolerable. One of the major problems in the simulation is in the evaluation of the vapour rate. The quasi steady state assumption made to calculate the vapour rate does not appear to be unrealistic for this particular column and perhaps should be considered in every case since it reduces the number of differential equations by a third. An alternative method has also been suggested in Chapter IV which relates the vapour rate to the pressure drop coefficient assuming it to be available. If the pressure drop coefficient is not available, the best method would probably be to integrate the component balance to obtain new values of x and hence y, T and the liquid and vapour stream

enthalpies. Assuming that the change in the enthalpy is small compared with the heat fluxes, an estimate of the enthalpy derivative (dh/dt) may be obtained from the energy balance equation at the latest integration step. The energy balance equation can then be rearranged to obtain the vapour rate on each tray starting from the reboiler.

During the experimental verifications of the column simulation, the predicted tray temperatures differed from the actual ones by ±0.6 of a degree centigrade under steady state and transient conditions. This discrepancy is thought to be due to

(i) the measurement errors : the following measurements are necessary:

(a) feed rate and composition

(b) reflux rate

(c) feed and reflux temperatures

(d) heat input rate

(e) reflux drum and reboiler holdups

Of these only the flow rate measurements were not particularly accurate. Since the column response is relatively more sensitive to these variables than others, they are suspected to have made the largest contributions to the discrepancy between the predicted and actual temperatures

(ii) the inaccuracies in the prediction of tray efficiencies which is partly due to the fact

that the physical properties are all determined by predictive methods

(iii) the inaccuracies of the estimation of heat losses

(iv) the assumption of 100 per cent equilibrium efficiency at the reboiler. A more exact value obtained experimentally would have produced better results

(v) the assumption of constant pressure is not strictly true. The pressure at the reboiler is higher than the top. Two pressure measurements would enable better comparison

Since the holdups in the reflux drum and the reboiler are considerably larger than that of a typical tray, it was not unrealistic to assume perfect level control at these points which is again consistent with the philosophy of replacing the differential equations by their steady-state approximations when possible. In practice, tight level controllers will enable the levels to remain almost constant and because of large holdups, the minor variations in them are ironed out.

IX.4 ESTIMATION

The proposed methodology for the extension of the linear Kalman filter to nonlinear systems appears to have overcome the typical stability problems reported in the literature. Chemical engineering systems as nonlinear as distillation with highly nonlinear measurement functional relationships are rare - although a few pathological cases may be cited. Therefore, it is questionable whether further extension of linear filtering theory such as adaptive filtering is justifiable for chemical processes - especially in complex high dimensionality systems.

As regards the binary distillation case, the performance of the filter model (Model I based on mass balances only) has been compared with that of the column simulator (Model II) in Chapter V. It can be seen that the filter model predictions are very inaccurate. The assumption of ideality has also been made in the derivation of the filter model for the measurement relationships which is again inaccurate. Despite these inbuilt approximations in the filter models, the measurement noise and the erratic deterministic disturbances of known and unknown natures, the extended Kalman filters formulated in this research produced accurate estimates of the state of the column from a handful of corrupt temperature measurements with sample times of up to 40 seconds. The filters were also insensitive to the integration method

used for predictions. They were equally accurate and stable with the simple Euler while the column simulator was being integrated by the fourth-order Runge-Kutta method - the step sizesbeing equal.

Dynamic simulation studies with the column simulator and extensive print-outs have pointed to the fact that the assumption of constant tray holdups does not appear to be unreasonable. Therefore, the order of the filter's system model can be decreased by a half if it is formulated based on this assumption. This means less intersample calculations, hence smaller sample times and more accurate estimates. This can be an important corollary especially in larger columns where adequate low order filter models are needed.

Finally, the ability of extended Kalman filters to function as fast and accurate on-line analysers opens interesting possibilities for overcoming hardware problems by the relatively inexpensive software approach - especially in relation to control.

IX.5 ESTIMATOR-AIDED FEEDFORWARD CONTROL

The simulation results have shown that the performance of EAFF control is superior to feedback temperature control in that

(i) when the column is subjected to a sustained step increase in the feed rate, the controlled variables undergo less transients and take far less time to return to their desired setpoints (see Figures VIII.5 and VIII.6)

(ii) the IAE for EAFF control is half as much as that for feedback temperature control even when the feedback controllers are tightly tuned

(iii) when the column was subjected to multiple disturbances under feedback temperature control in a subsequent experiment (see Figures VIII.9 and VIII.10), the column became unstable pointing to the fact that the tuning of these controllers was too tight in the previous experiment to make their associated IAE, used for comparison with that of EAFF control, representative and meaningful. In real life one would not risk tuning the controllers so tightly and, therefore a much larger IAE would be expected. Even under these conditions, the performance of EAFF control was twice as good as feedback control.

(iv) EAFF control appears to be more efficient in terms of finding the right targets for the

manipulated variables (Figures VIII.7, VIII.8, VIII.11 and VIII.12) when known and unknown disturbances do occur. This primarily means that EAFF control minimizes the typical interaction problems experienced with feedback control. This is to be expected because of its self-corrective nature. Secondly, in terms of energy consumption and producing less off-specification compositions, EAFF control is superior to feedback temperature control

Therefore, EAFF control may offer a plausible approach to meeting the recent criticisms raised against the status of chemical process control.

In the example used as the test case, the same model was used for predicting the state variables for estimation and for control. If, however, having calculated the predicted state at the next sample time and having computed the control inputs, the filter's system model is reintegrated with the new values of the control inputs for estimation, the state estimation should be more accurate and so should the control. Obviously, this proposal can only be implemented if there is sufficient time in between samples to perform the state predictions twice, once for control and once for estimation.

Another important consideration in the design of extended Kalman filters for EAFF control is that all of the control inputs should be estimated as parameters and measured if possible.

IX.6 RECOMMENDATIONS FOR FURTHER WORK

As regards hardware modifications to the distillation column a number of proposals have already been made.

As far as the theoretical proposals are concerned, and in relation to distillation, the logical extension of this work would be to test these ideas on multicomponent distillation whether they be related to simulation, estimation or control.

EAFF control could be tested on other well-understood multivariable systems such as chemical reactors with controllers preferably designed by a multivariable feedforward design method. The publications of the University of Alberta in Canada (102) provide a good survey of the available multivariable design methods.

A P P E N D I X A

A.1 THE CHARACTERISTICS OF THE MOTORIZED VALVES

The valve positions have been tabulated against their corresponding digital output channel numbers in the following table.

Digital Output Channel Number	Position of the Valve	Characteristic Figure Number
1	Reflux	A.1.1
2	Bottoms	A.1.2
3	Feed	A.1.3
4	Distillate	A.1.4
5	Condenser cooling water	Not studied

The characteristic equations are given in Chapter III, in Table III.3.

Figure A.1.1

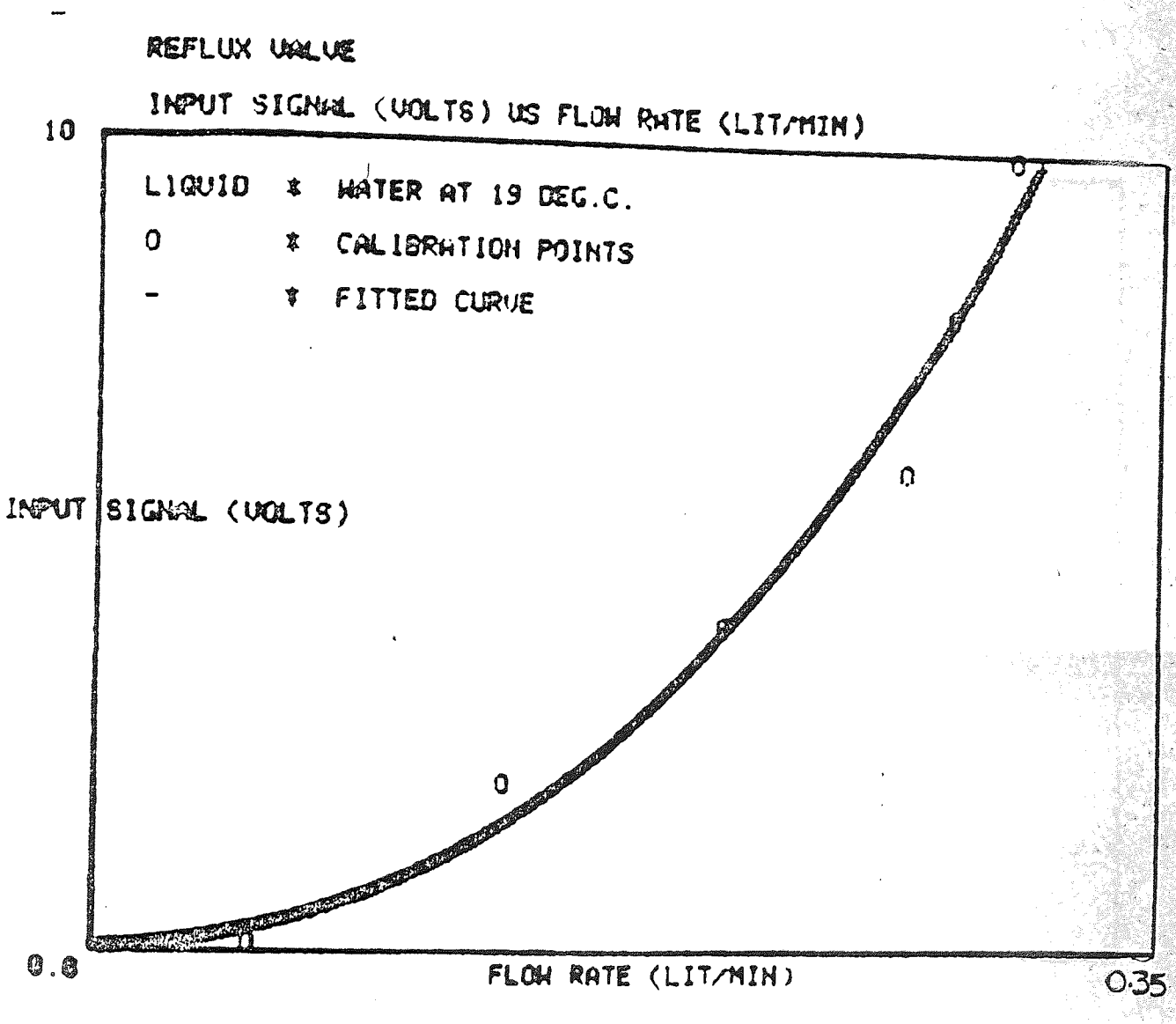

REFLUX VALVE
INPUT SIGNAL (VOLTS) VS FLOW RATE (LIT/MIN)
10
LIQUID * WATER AT 19 DEG.C.
0 * CALIBRATION POINTS
- * FITTED CURVE
INPUT SIGNAL (VOLTS)
0.0
FLOW RATE (LIT/MIN)
0.35

Figure A.1.2

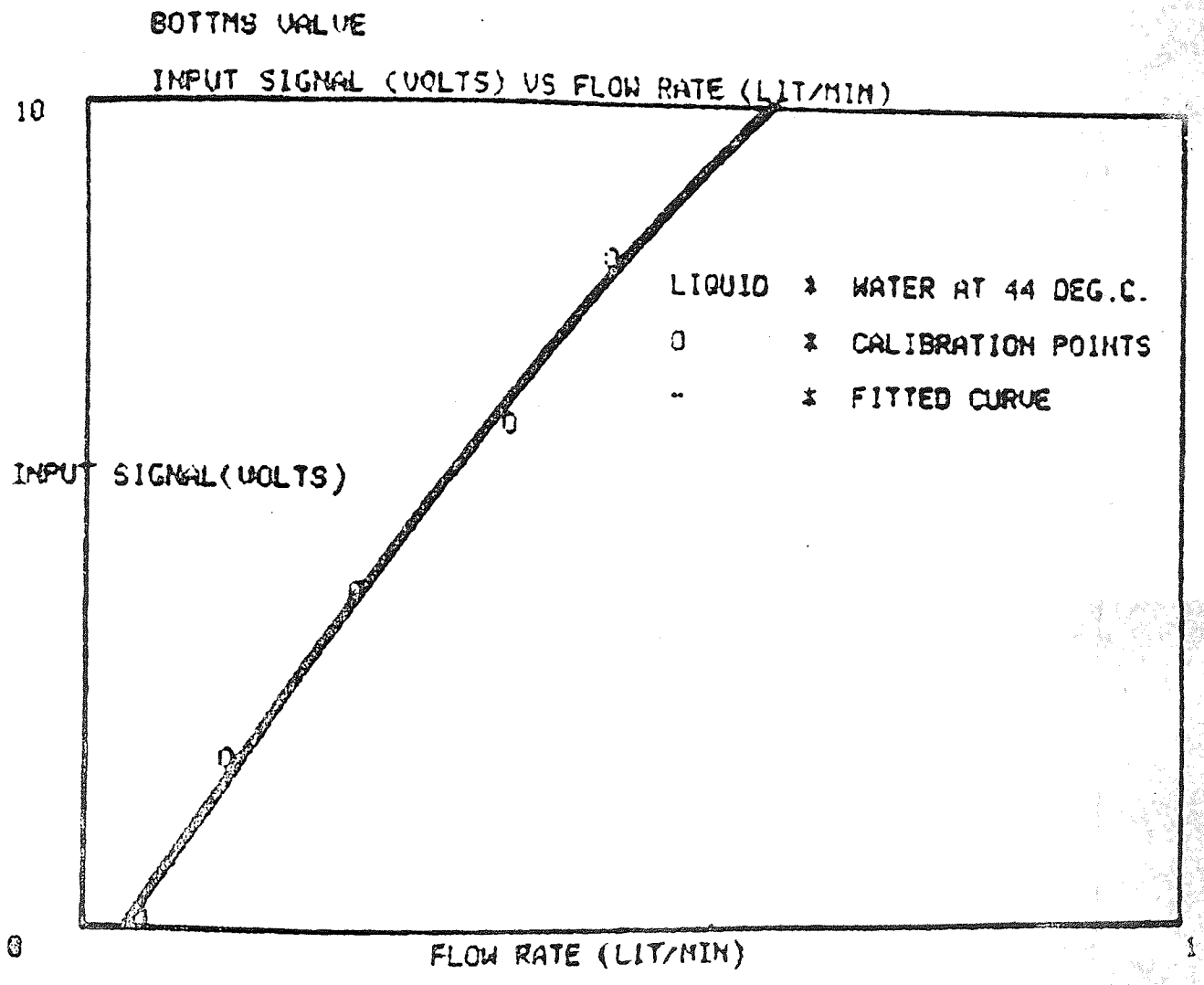

BOTTMS VALVE
INPUT SIGNAL (VOLTS) VS FLOW RATE (LIT/MIN)
10
INPUT SIGNAL(VOLTS)
0
FLOW RATE (LIT/MIN)
1
LIQUID * WATER AT 44 DEG.C.
O * CALIBRATION POINTS
- * FITTED CURVE

Figure A.1.3

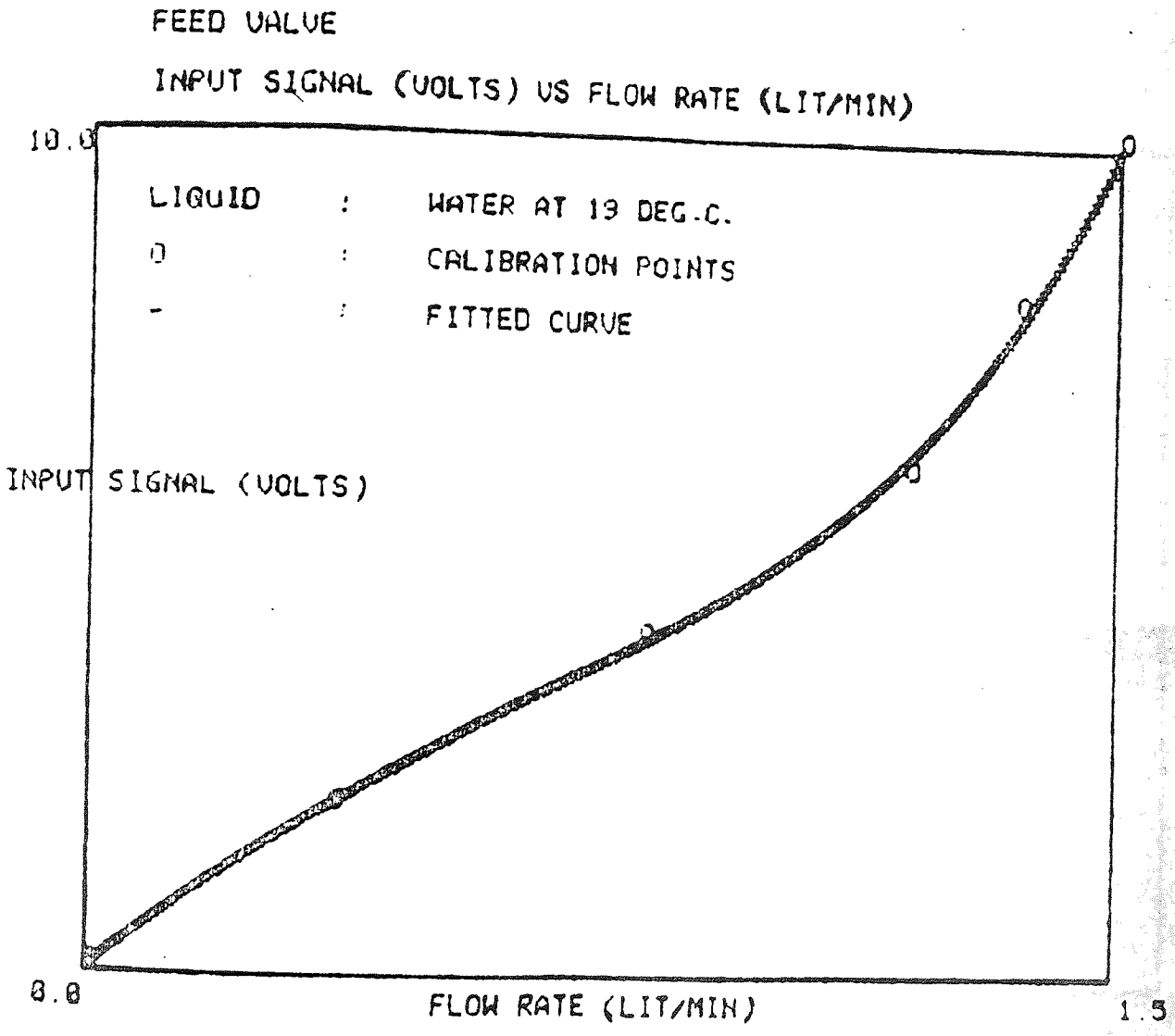
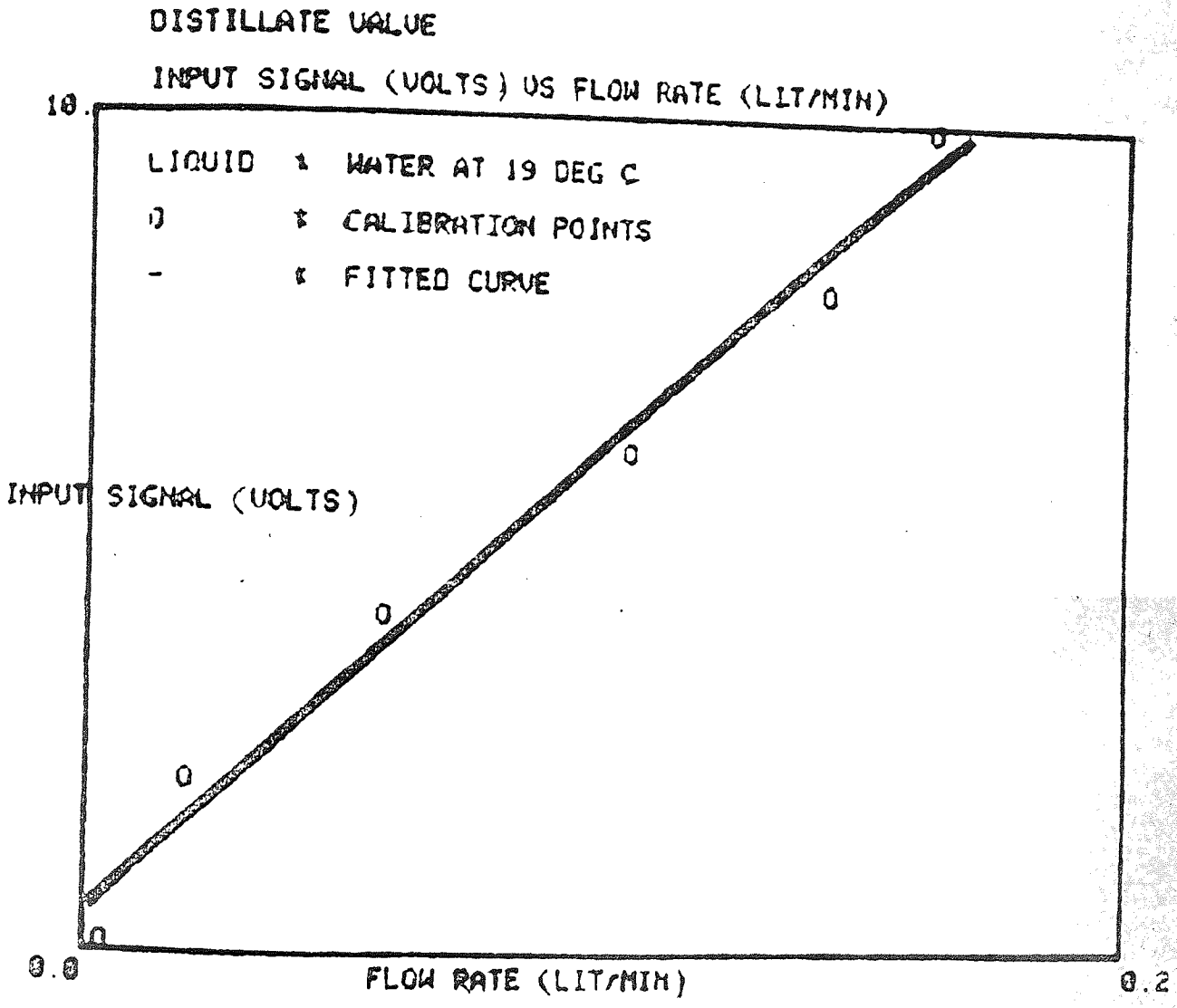

FEED VALVE
INPUT SIGNAL (VOLTS) VS FLOW RATE (LIT/MIN)
10.0
LIQUID : WATER AT 13 DEG.C.
O : CALIBRATION POINTS
- : FITTED CURVE
INPUT SIGNAL (VOLTS)
0.0
FLOW RATE (LIT/MIN)
1.5

Figure A.1.4


DISTILLATE VALUE
INPUT SIGNAL (VOLTS) VS FLOW RATE (LIT/MIN)
10.
LIQUID : WATER AT 19 DEG C
0 : CALIBRATION POINTS
- : FITTED CURVE
INPUT SIGNAL (VOLTS)
0.0
FLOW RATE (LIT/MIN)
0.2

A.2 THE REBOILER CHARACTERISTICS

The digital output channel number 6 corresponds to the reboiler. The characteristic curves for the reboiler are as follows:

Figure A.2.1 : Q_{12} vs input signal

Figure A.2.2 : input signal vs Q_{12}

Figure A.2.3 : heat transfer rate vs mass of liquid in the reboiler

Figure A.2.4 : $R = \frac{Q_{12}}{Q_A}$ vs mass of liquid in the reboiler

where

Q_A = actual heat transfer rate

Q_{12} = heat transfer rate when the reboiler holdup is 12 kg.

Figure A.2.1

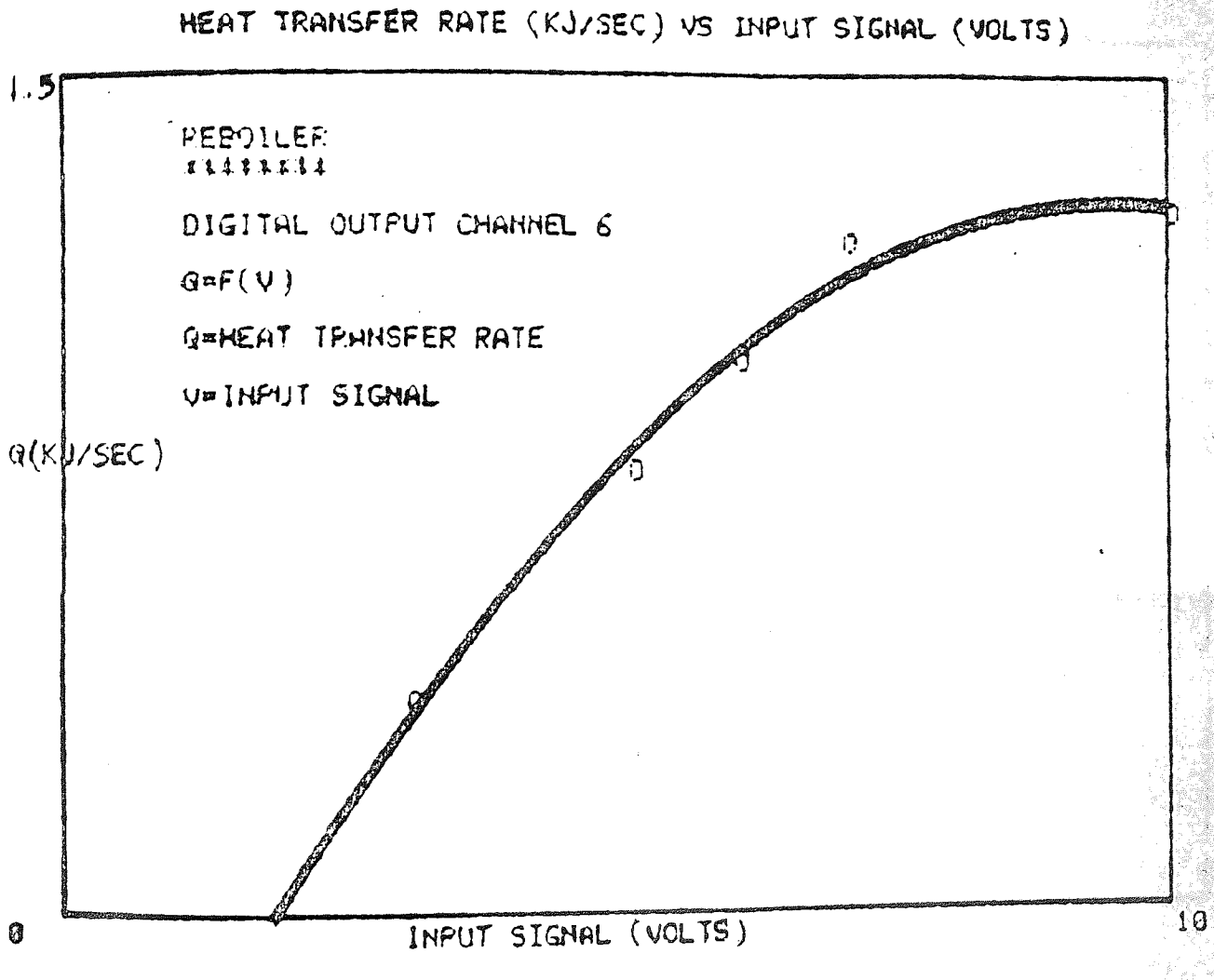

HEAT TRANSFER RATE (KJ/SEC) VS INPUT SIGNAL (VOLTS)
1.5
REBOILER
DIGITAL OUTPUT CHANNEL 6
Q=F(V)
Q=HEAT TRANSFER RATE
V=INPUT SIGNAL
Q(KJ/SEC)
0
INPUT SIGNAL (VOLTS)
10

Figure A.2.2

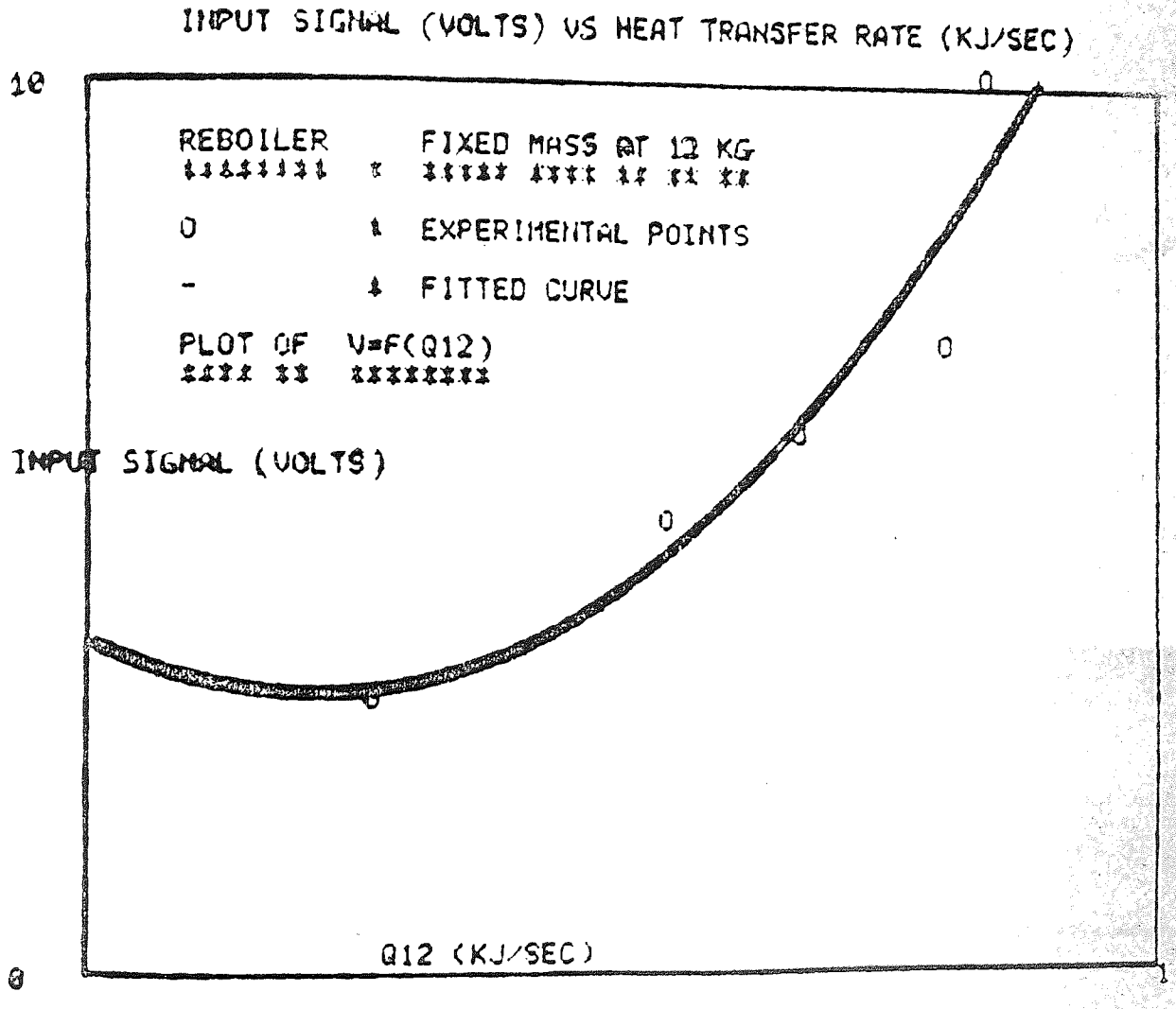

INPUT SIGNAL (VOLTS) VS HEAT TRANSFER RATE (KJ/SEC)
10
REBOILER
FIXED MASS AT 12 KG
EXPERIMENTAL POINTS
FITTED CURVE
PLOT OF V=F(Q12)
INPUT SIGNAL (VOLTS)
Q12 (KJ/SEC)
0

Figure A.2.3

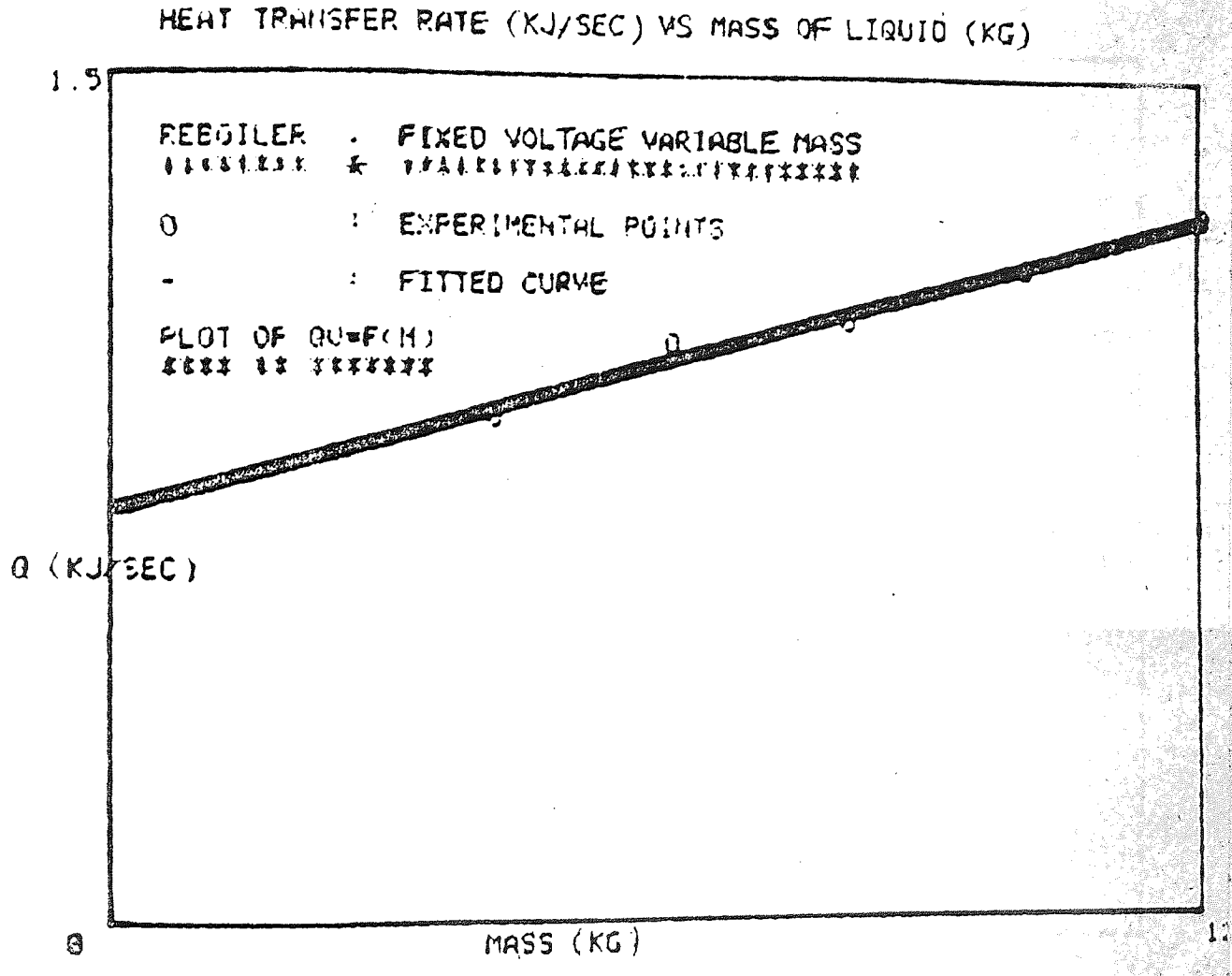
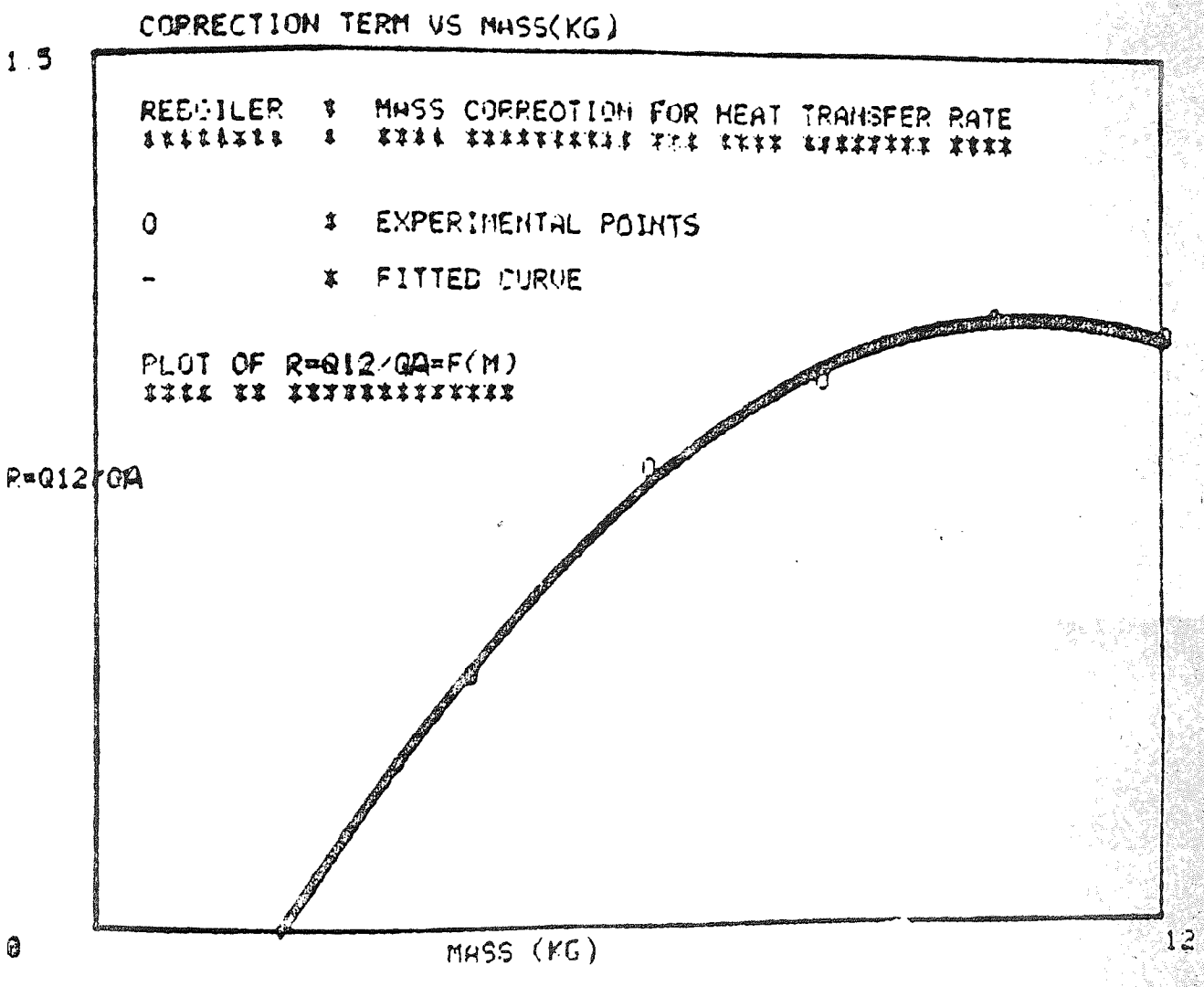

HEAT TRANSFER RATE (KJ/SEC) VS MASS OF LIQUID (KG)
1.5
REBOILER . FIXED VOLTAGE VARIABLE MASS
O : EXPERIMENTAL POINTS
- : FITTED CURVE
PLOT OF QU=F(M)
Q (KJ/SEC)
0
MASS (KG)

Figure A.2.4


CORRECTION TERM VS MASS(KG)
1.5
REBOILER * MASS CORRECTION FOR HEAT TRANSFER RATE
0 * EXPERIMENTAL POINTS
- * FITTED CURVE
PLOT OF R=Q12/QA=F(M)
R=Q12/QA
0
MASS (KG)
12

A.3 THE THERMOCOUPLE CHARACTERISTICS

The characteristic equations have been given in Chapter III.

Figure Number	Correlated Variables	Process Variable Measured
A.3.1	T vs V	Top tray temperature
A.3.1	T vs V	Feed tray temperature
A.3.2	T vs V	Bottom tray temperature

where T denotes temperature in ^{o}C.

V refers to output voltage from the thermocouple in volts

Figure A.3.1

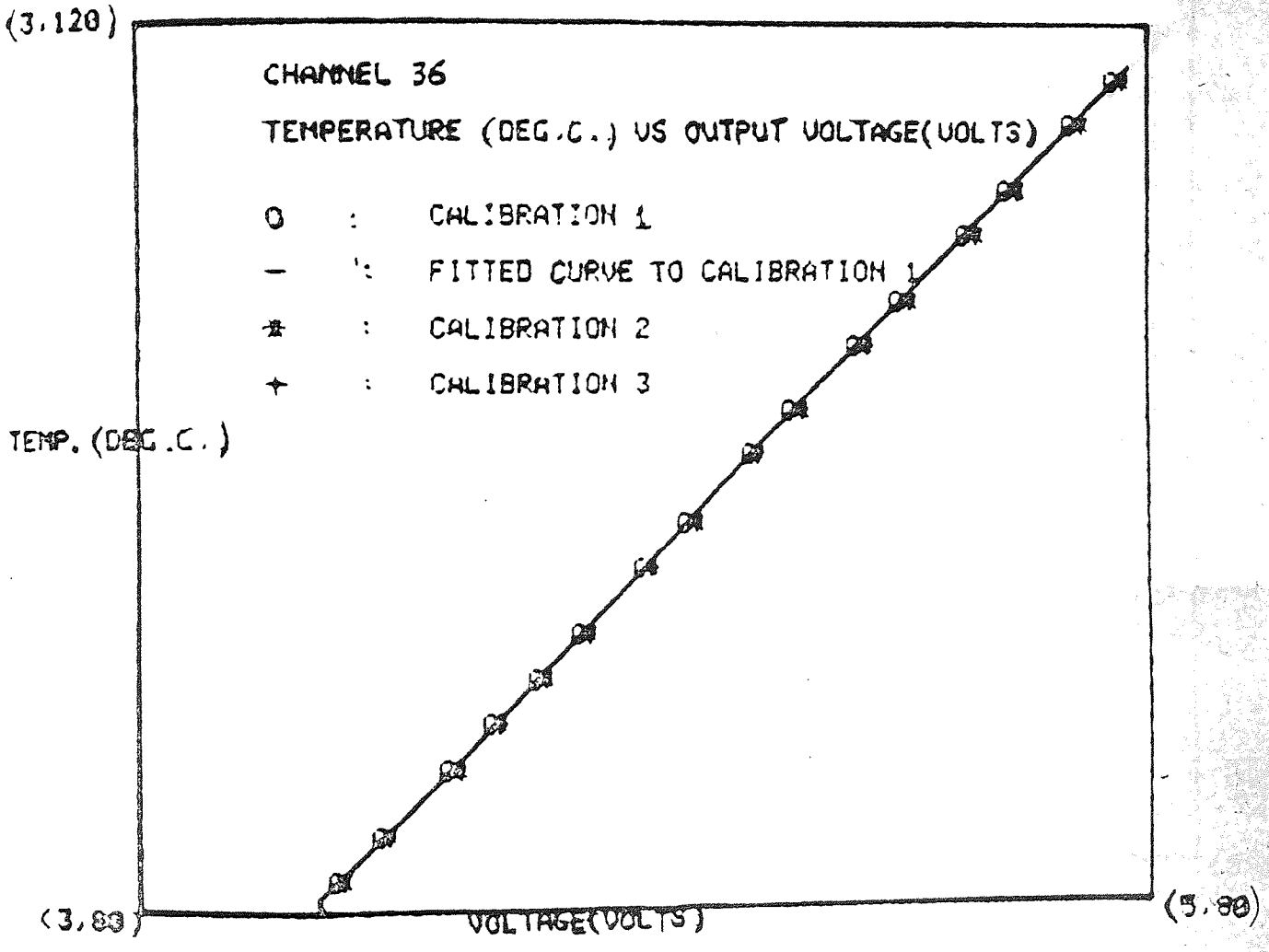

(3,120)
CHANNEL 36
TEMPERATURE (DEG.C.) VS OUTPUT VOLTAGE(VOLTS)
O : CALIBRATION 1
— : FITTED CURVE TO CALIBRATION 1
✱ : CALIBRATION 2
✦ : CALIBRATION 3
TEMP. (DEG.C.)
(3,80)
VOLTAGE(VOLTS)
(5,80)

Figure A.3.2

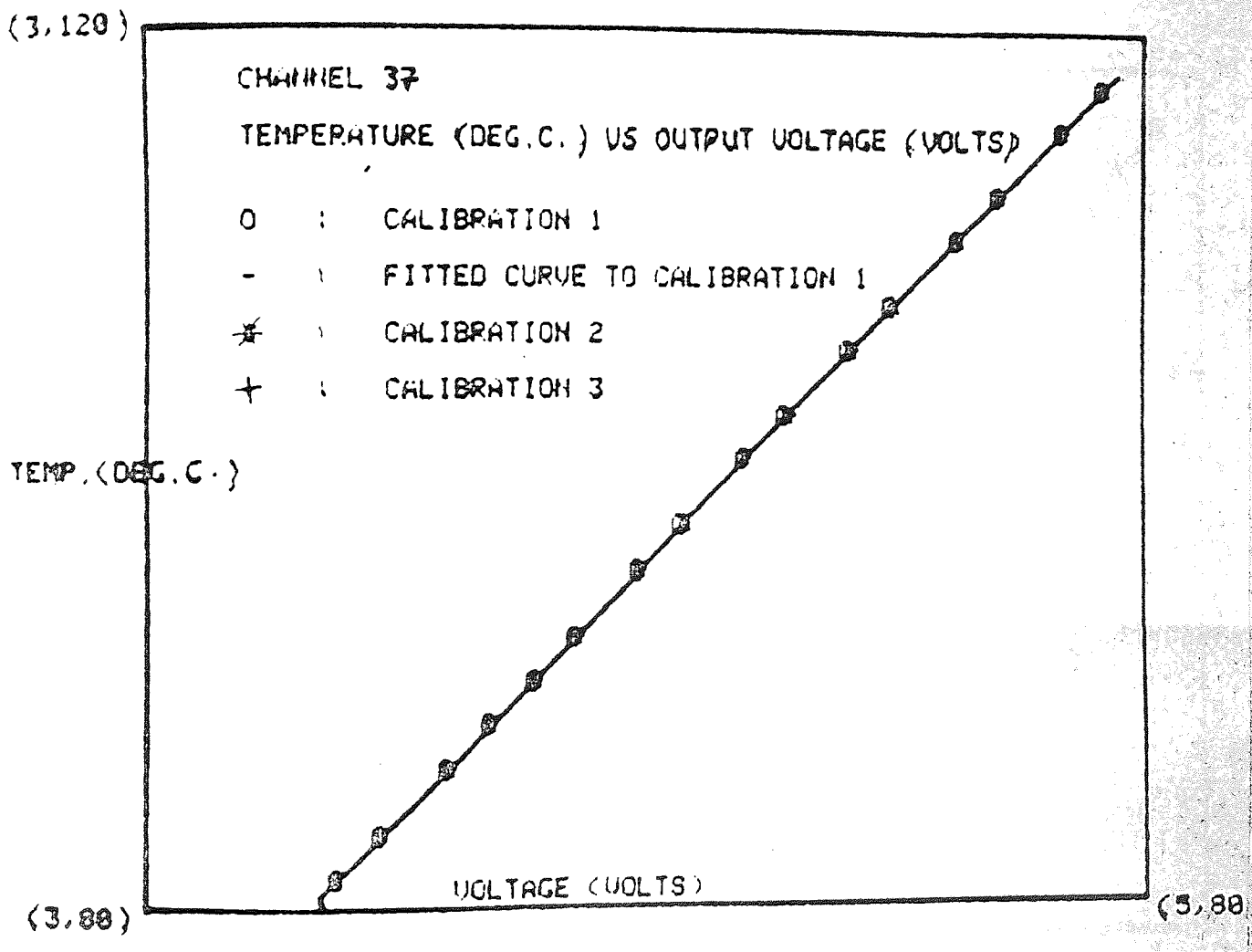
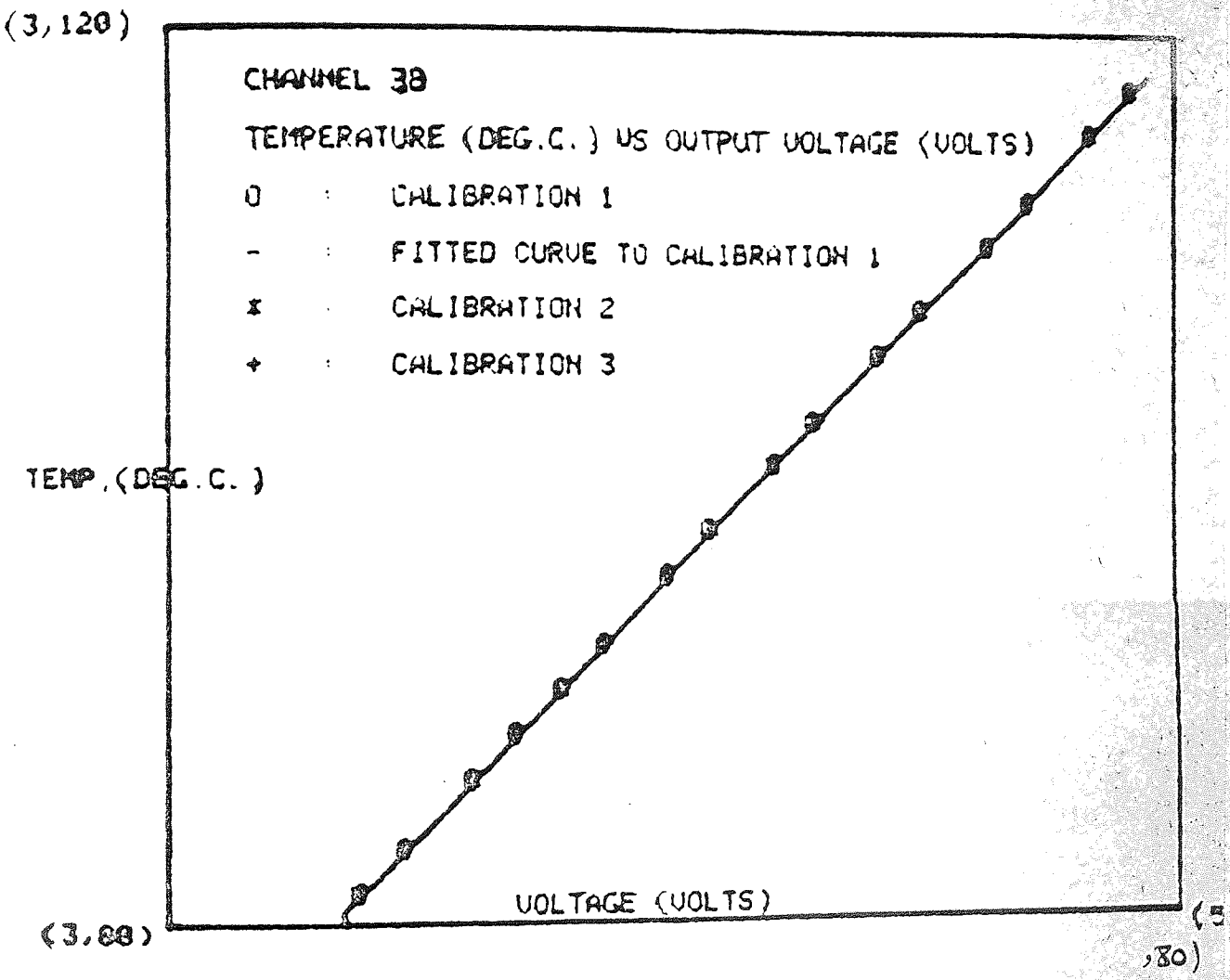

(3,120)
CHANNEL 37
TEMPERATURE (DEG.C.) VS OUTPUT VOLTAGE (VOLTS)
O : CALIBRATION 1
- : FITTED CURVE TO CALIBRATION 1
CALIBRATION 2
CALIBRATION 3
TEMP.(DEG.C.)
VOLTAGE (VOLTS)
(3,80)
(5,80)

Figure A.3.3


(3,120)
CHANNEL 38
TEMPERATURE (DEG.C.) VS OUTPUT VOLTAGE (VOLTS)
0 : CALIBRATION 1
- : FITTED CURVE TO CALIBRATION 1
x : CALIBRATION 2
+ : CALIBRATION 3
TEMP.(DEG.C.)
VOLTAGE (VOLTS)
(3,80)
,80)

A.4 THE CHARACTERISTICS OF THE LEVEL-INDICATORS

Figure A.4.1 : The reflux drum level indicator

Figure A.4.2 : The reboiler level-indicator

Figure A.4.1

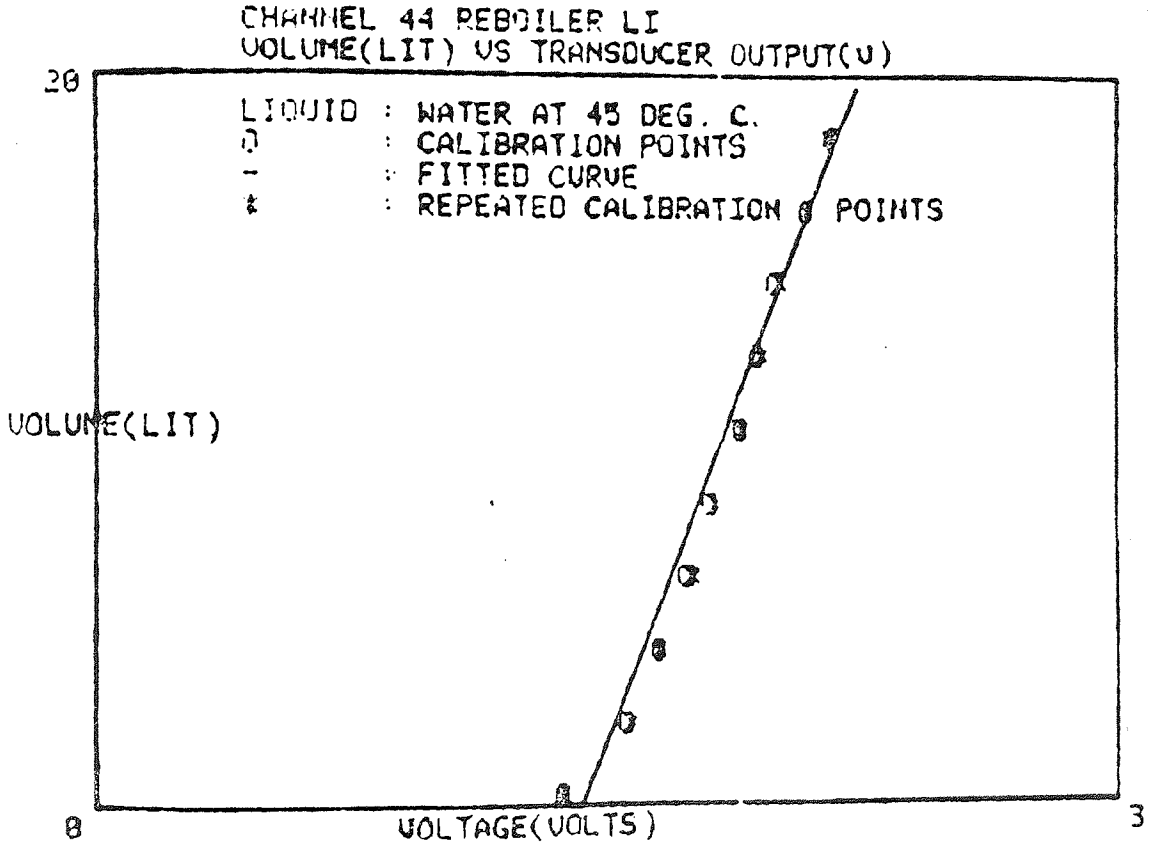
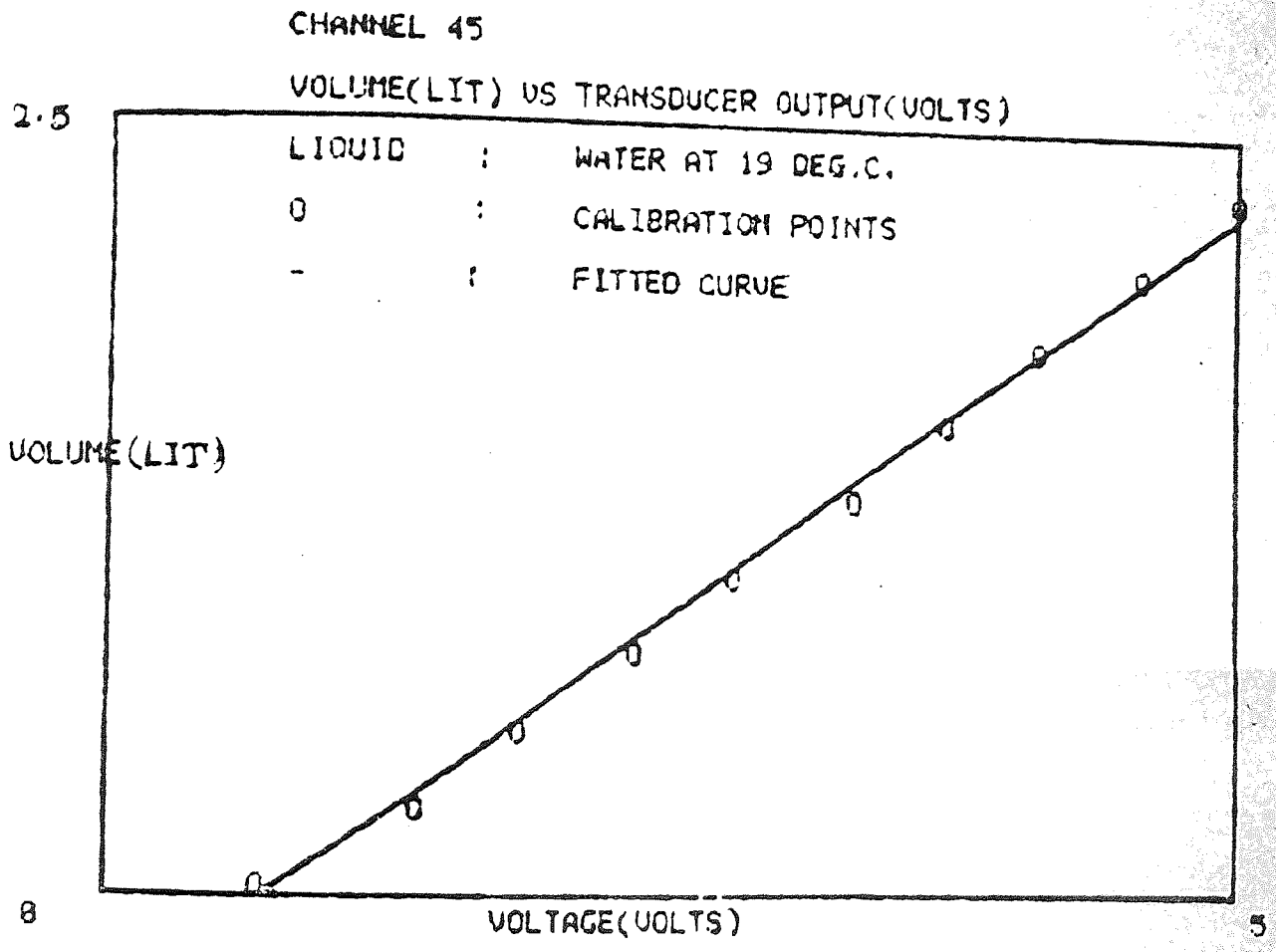

CHANNEL 44 REBOILER LI
VOLUME(LIT) VS TRANSDUCER OUTPUT(V)
20
LIQUID : WATER AT 45 DEG. C.
O : CALIBRATION POINTS
- : FITTED CURVE
* : REPEATED CALIBRATION POINTS
VOLUME(LIT)
0
VOLTAGE(VOLTS)
3

Figure A.4.2


CHANNEL 45
VOLUME(LIT) VS TRANSDUCER OUTPUT(VOLTS)
LIQUID : WATER AT 19 DEG.C.
0 : CALIBRATION POINTS
- : FITTED CURVE
2.5
VOLUME(LIT)
0
VOLTAGE(VOLTS)
5

A.5 THE FLOW MEASUREMENT TRANSDUCER CHARACTERISTICS

Figure A.5.1 : feed rate measurement

Figure A.5.2 : bottoms measurement

Figure A.5.3 : distillate measurement

Figure A.5.4 : reflux rate measurement

A.5.1 THE ORIFICE PLATE HOLE SIZES

Measurement	Orifice Size
Feed	1.8 mm
Bottoms	2.0 mm
Distillate	1.3 mm
Reflux	1.3 mm
Condenser cooling water	5.0 mm

The sizes of the orifice holes have been chosen by trial and error. The following considerations are instrumental in the choice of these hole sizes:

(i) they must be small enough to give the right sensitivity

(ii) they have to be sufficiently large in order not to flood the transducers at the maximum openings of their associated motorized valves

A.5.2 CALIBRATION EQUATIONS

The form of the correlation is

$$F = a + bv + cv^2 + dv^3$$

where

F = flow rate cc./min.

v = transducer output volts

α = correlation coefficients

a,b,c,d = constants

The polynomial coefficients are tabulated below.

Flow	a	b	c	d	α
Reflux	-10.2	81.9	-	-	0.91
Bottoms	46.2	135.0	-	-	0.94
Feed	-128	590	-75.4	-	0.97
Distillate	-44.62	123.3	-26.87	2.409	0.92

The curve-fittings were done by the least squares method.

Figure A.5.1

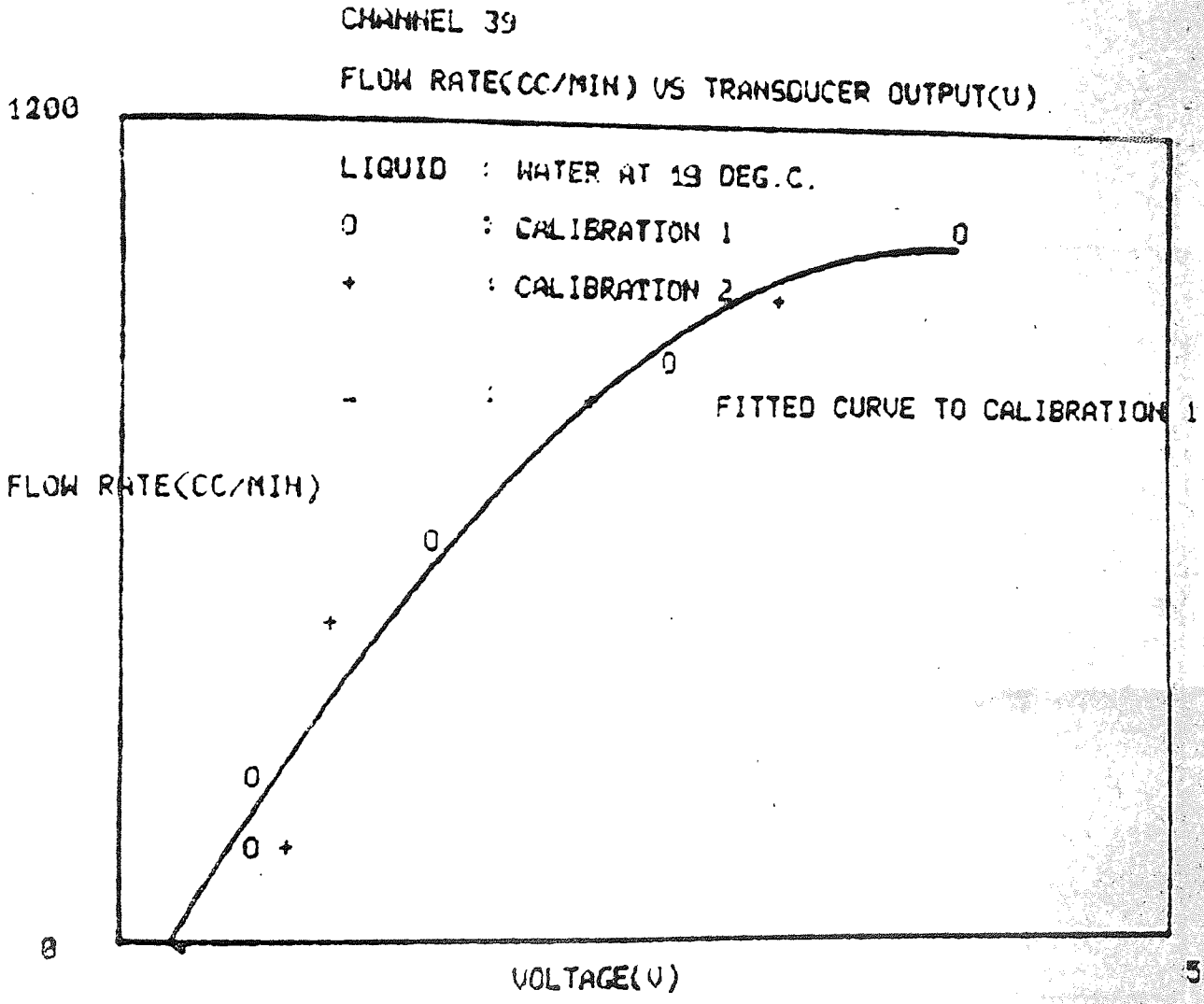

CHANNEL 39
FLOW RATE(CC/MIN) VS TRANSDUCER OUTPUT(V)
1200
LIQUID : WATER AT 19 DEG.C.
O : CALIBRATION 1
+ : CALIBRATION 2
- :
FITTED CURVE TO CALIBRATION 1
FLOW RATE(CC/MIN)
0
VOLTAGE(V)
5

Figure A.5.2

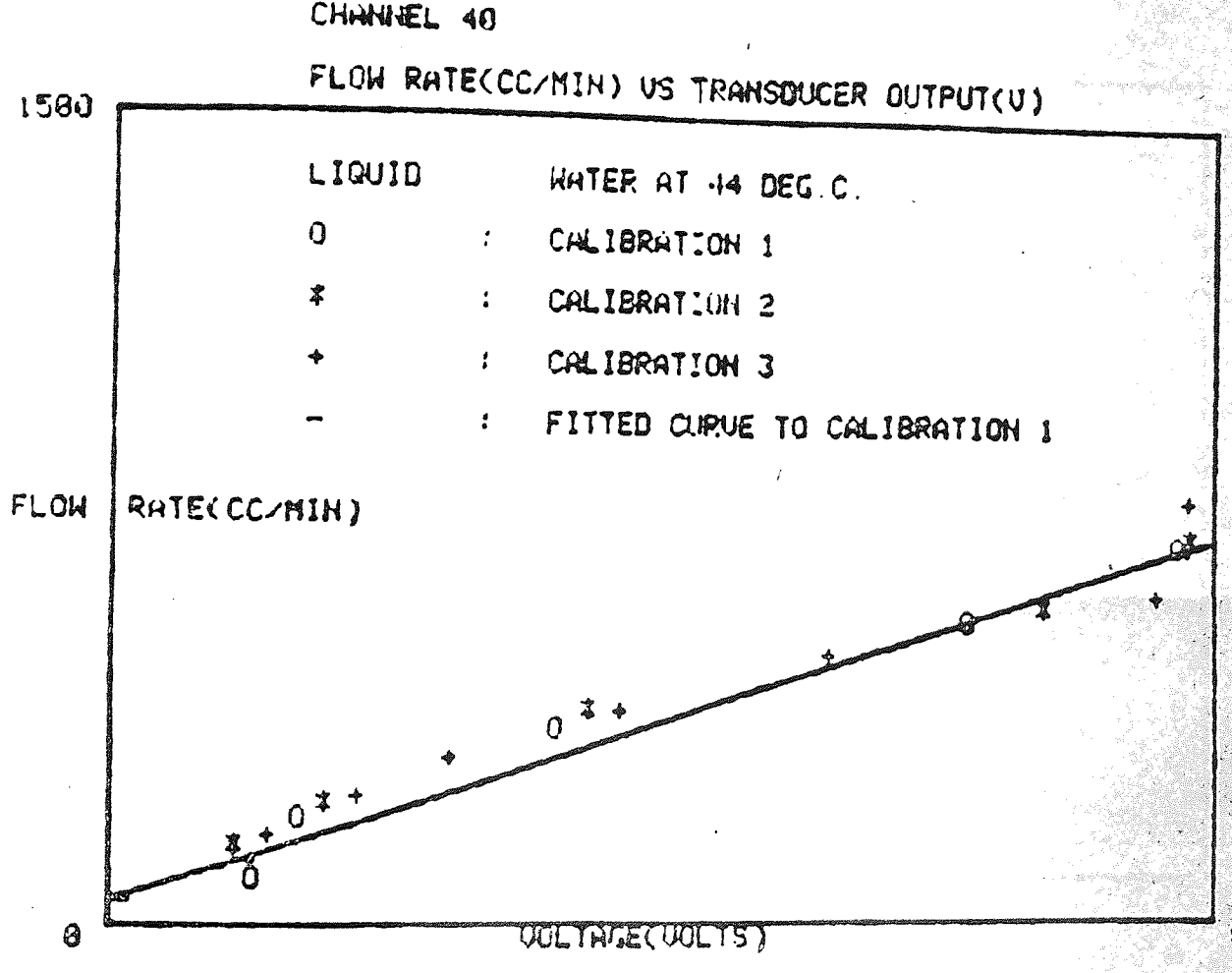

CHANNEL 40
FLOW RATE(CC/MIN) VS TRANSDUCER OUTPUT(V)
1500
LIQUID WATER AT 14 DEG.C.
O : CALIBRATION 1
* : CALIBRATION 2
+ : CALIBRATION 3
- : FITTED CURVE TO CALIBRATION 1
FLOW RATE(CC/MIN)
0
VOLTAGE(VOLTS)

Figure A.5.3

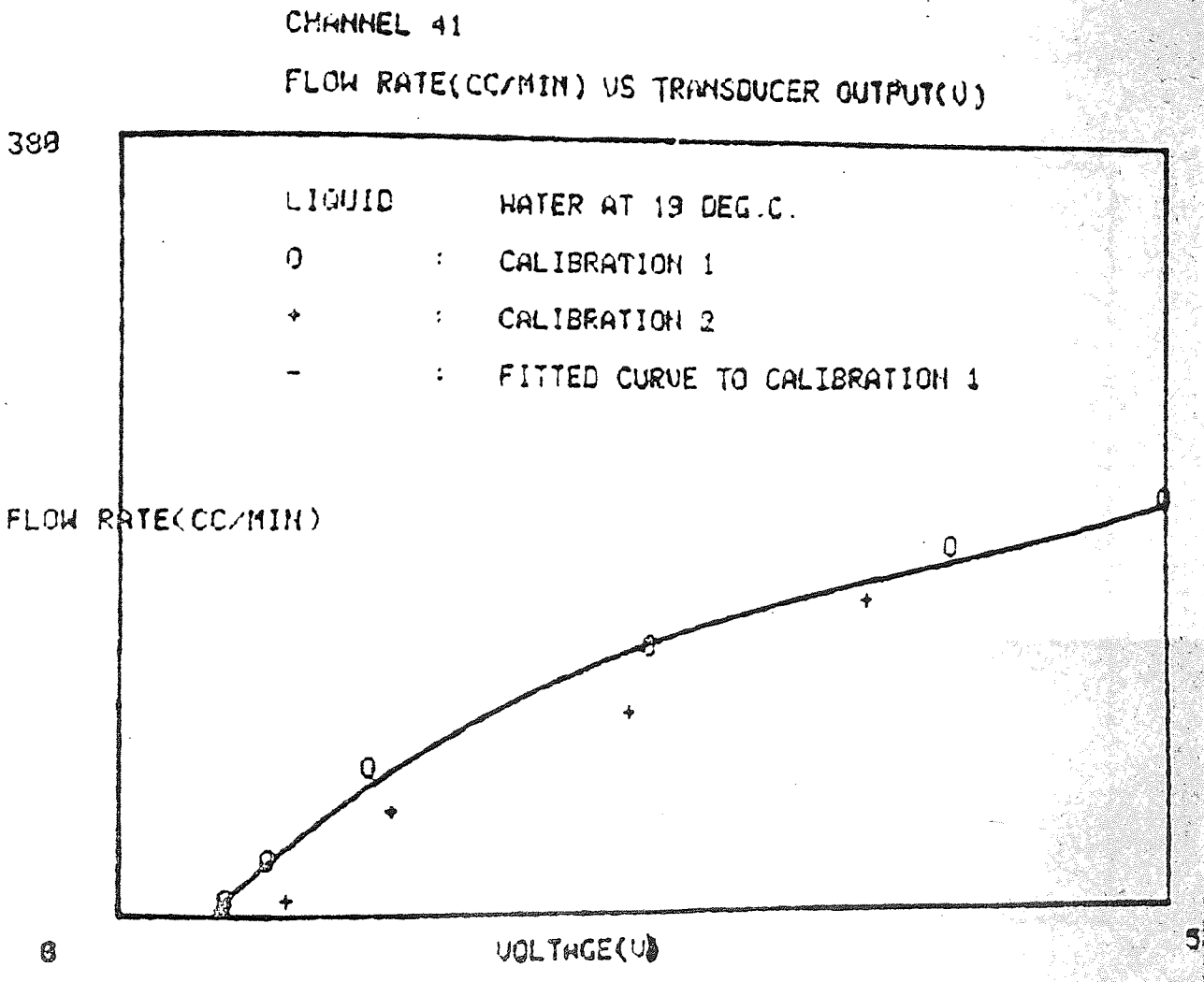
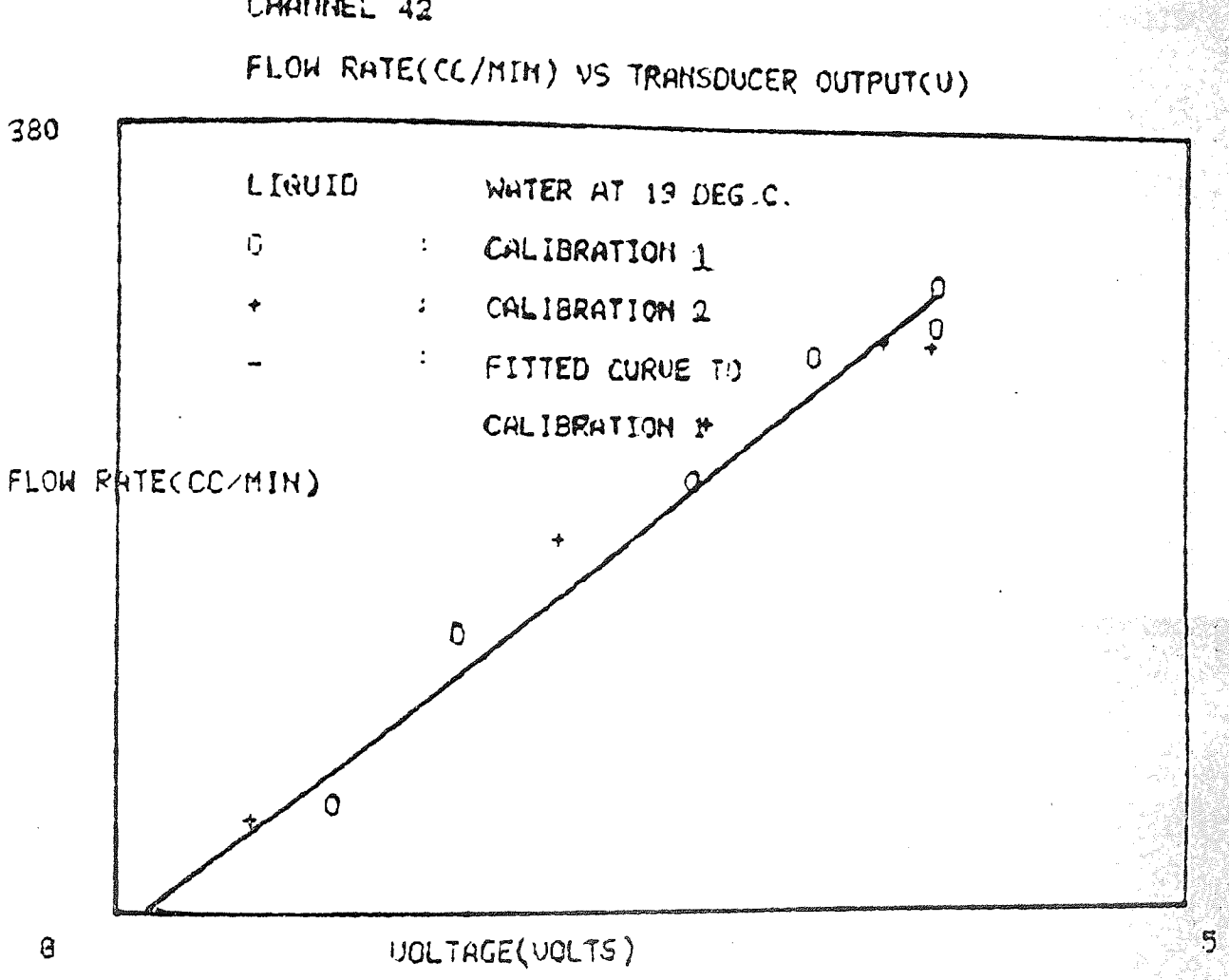

CHANNEL 41
FLOW RATE(CC/MIN) VS TRANSDUCER OUTPUT(V)
LIQUID WATER AT 19 DEG.C.
O : CALIBRATION 1
+ : CALIBRATION 2
- : FITTED CURVE TO CALIBRATION 1
FLOW RATE(CC/MIN)
300
0
VOLTAGE(V)
5

Figure A.5.4


CHANNEL 42
FLOW RATE(CC/MIN) VS TRANSDUCER OUTPUT(U)
380
LIQUID WATER AT 19 DEG.C.
O : CALIBRATION 1
+ : CALIBRATION 2
- : FITTED CURVE TO CALIBRATION *
FLOW RATE(CC/MIN)
0
5
VOLTAGE(VOLTS)

A P P E N D I X B

B.1 THE PROPOSED STRUCTURE FOR A PROCESS SIMULATOR

In a dynamic simulator, next to the mathematical modelling aspects, the role of the structure relative to that of the integrator is of central importance and has considerable bearing on the flexibility of the simulator. Unfortunately, most, if not all, of the available integrators require that a structure be set up in a predefined manner and that once the integrator is called, it will then take control of the operations without allowing any further user interference until the simulation is finished. In other words, the structure is subordinate to the integrator and must be designed to suit the integrator. This arrangement can be somewhat limiting and cumbersome since, ideally, one would like an integrator that can be called autonomously at any point within the structure to update any number of variables and report back at the end of any number of steps. Additionally, it is often helpful if the independent variable is advanced outside the integrator as the user desires as opposed to its being advanced by the integrator. This aspect can enhance the flexibility of the simulator especially for on-line applications where the chances of missing a sample or a control point will practically be zero since the user will have full control over advancing the time.

In order to enable the user to devise such a structure to suit his needs, a collection of four FORTRAN subroutines are proposed which are, namely,

SDINT, INTJS, INTPAS, and PRINT. Due to the important role of the integrator, some elaboration on the functions to be performed by these subroutines and an example of how the main program structure may be set up to communicate with this integrator will be in order at this stage.

SUBROUTINE SDINT

This subroutine carries out the integration and offers a choice of three different integration methods which are first-, second- and fourth-order respectively. These are as follows:

(i) the Euler method

(ii) the Euler predictor-corrector method

(iii) the Runge-Kutta method

Experience with a wide range of typical chemical engineering problems has shown that with almost no exception, the fourth-order Runge-Kutta method is quite adequate for any situation but the second- and first-order methods are also alternatives that can provide reasonable accuracy coupled with greater computational efficiency when short step sizes are forced on the Runge-Kutta.

The formal variables of this subroutine are:

(i) XX and DX; which contain the values of the integrated variable and its derivative respectively

(ii) TD; which represents the independent variable

(iii) DTD; which is the integration step size

(iv) IOD; which stands for the order of the integration

method

(v) INTCAL; when a set of differential equations are being solved simultaneously, this variable signals to the integrator which variable is being integrated so that the inter-step information corresponding to that variable can be identified in the higher order methods where more than one derivative evaluation is needed in each integration step

The common variables of this subroutine held in the COMMON block labelled INTEG are:

(i) JE; the integrator pass number for the Euler's method

(ii) JS; the pass number for the predictor-corrector method specifying whether the calculation is performing its first or second derivative evaluation

(iii) JS4; the pass number for the fourth-order Runge-Kutta method

(iv) ND; the total number of differential equations

SUBROUTINE INTJS

When a set of differential equations are being solved simultaneously, the function of this subroutine is to ensure that all of the dependent integrated variables are updated before the integrator pass number is advanced in the higher order integration methods (the predictor-corrector and Runge-Kutta fourth order).

The formal variables of this subroutine are:

(i) JS4,JS,JE and ND; as defined before.

(ii) IPASS; which is a flag for checking for the step completion in the higher order methods and is controlled by subroutine INTPAS. E.g. when JS4 is greater than 4, IPASS will be set to zero.

The common variables are as those defined for the subroutine SDINT.

SUBROUTINE PRINT

The purpose of this subroutine is to print variables of interest and also to control the frequency of printing. The number of variables that need to be printed is a problem-dependent consideration. These variables can be transferred to the subroutine through the argument list, or otherwise, and the corresponding WRITE statement can then be modified accordingly. This subprogram also safeguards against printing redundant interstep information by checking the integration pass numbers JS and JS4 when higher order integration methods are being used.

The formal variables of this subroutine are:

(i) T; is the independent variable

(ii) DT; is the integration step length

(iii) PI; is the print interval which should be equal to N*DT with N being an integer

(iv) plus any other variable of interest that needs to be printed out.

AN EXAMPLE

Consider a system represented by the following differential equation:

$$\ddot{y} + y = 0; \quad t=0,\ \dot{y}(0)=1.0,\ y(0)=0$$

This equation can be reduced to a set of two first order differential equations which can then be solved simultaneously. The program listing that follows shows the main program arrangement required to simulate this system and also the layout of the subprogram named DYMOD where the actual simulation takes place. This particular problem happens to have an analytical solution as well which is evaluated in subroutine ANMOD to enable comparison between the analytical and numerical solutions. The results are shown in Table B.1. As expected, for the same step size, higher order integration methods provide better accuracy.

GENERAL ARRANGEMENT OF THE MAIN PROGRAM FOR THE USE OF SDINT SUBROUTINES

The main program arrangement is depicted in Figure IV.1 in Chapter IV. Following a preliminary housekeeping section containing FORMATS and DECLARATION statements, the initialization section is laid out. Here all the calculations and specification for the problem parameters and coefficients are made. These are the values that are normally invariant during the course of the calculations. In this section, the initial conditions for the integrated variables must also be specified. The next section is the dynamic section in which the individual simulator modules are called to perform the simulation and the independent variable is advanced when all the modules have been updated.

THE PROGRAM ARRANGEMENT FOR THE INDIVIDUAL SIMULATOR MODULES

The individual simulator modules must be laid out according to the flowchart shown in Figure IV.2. Each module essentially comprises:

(i) the preliminary calculation section (if necessary)

(ii) the derivative section in which the derivatives are defined

(iii) the integration section where the dependent variables are updated

(iv) the test for the step completion and a CALL to the subroutine INTPAS to zero the integrator pass numbers for the next step

```
C:::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
C:     PROGRAM TO TEST THE FIXED STEP INTEGRATOR AND THE
C:     PROPOSED STRUCTURE
C:     EXAMPLE 1 ; SOLUTION OF A 2ND ORDER O.D.E                        :
C:                          *** SYMBOLS ***                             :
C:     Z=VECTOR OF SOLUTIONS FOUND BY NUMERICAL INTEGRATION             :
C:    AZ=VECTOR OF ANALYTICAL SOLUTIONS                                 :
C:    DZ=VECTOR OF DERIVATIVES                                          :
C:  TIME=THE INDEPENDENT VARIABLE                                       :
C:    PI=PRINT INTERVAL ; AN INTEGER MULTIPLE OF DT                     :
C:    DT=STEP LENGTH
C:IPASS=INTEGRATOR PASS NUMBER                                          :
C:   IOD=INTEGRATION ORDER                                             :
C:       =1     EULER                                                  :
C:       =2     PREDICTOR CORRECTOR                                    :
C:       =4     RUNGE-KUTTA FOURTH ORDER                               :
C:    JE=FLAG FOR STEP COMPLETION IN EULER                              :
C:    JS=FLAG FOR STEP COMPLETION IN PREDICTOR-CORRECTOR                :
C:   JS4=FLAG FOR STEP COMPLETION IN RUNGE-KUTTA                       :
C:    ND=NUMBER OF DIFFERENTIAL EQUATION IN EACH MODULE                 :
C:ANMOD=SIMULATOR MODULE USING ANALYTICAL SOLUTIONS                     :
C:DYMOD=SIMULATOR MODULE USING NUMERICAL  SOLUTIONS                     :
C:::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::::
      COMMON/MODEL/Z(2),AZ(2),DZ(2),A,B
      COMMON/INTEG/JS4,JS,JE,ND
C**** INFORMATION NEEDED FOR THE INTEGRATOR
      JE=0
      JS=0
      JS4=0
      READ(1,100) DT,PI,ENDT,IOD
  100 FORMAT(3F0.0,1I0)
      ND=2
      IPASS=0
C**** CONSTANTS
      READ(1,200) A,B
  200 FORMAT(2F0.0)
C**** INITIALIZATION
      TIME=0.
      Z(1)=0.
      Z(2)=1.
      AZ(1)=0.
C**** PRINT TITLE
      WRITE(2,1)
    1 FORMAT(3X,'TIME',8X,'AZ ',8X,'Z ',8X,'ERROR'/
     +,      3X,'****',8X,'**',9X,'*',7X,'*****')
C**** DYNAMIC SECTION
    2 CONTINUE
      CALL PRINT(TIME,DT,PI,AZ,Z)
      CALL DYMOD(TIME,DT,IOD)
      CALL ANMOD(TIME,ND)
      IF(TIME.GT.ENDT)      GO TO 3
      TIME=TIME+DT
      GO TO 2
    3 CONTINUE
C**** END OF SIMULATION
      STOP
      END
```

```
C**** PRINT SUBROUTINE
      SUBROUTINE PRINT(T,DT,PI,AZ,Z)
      DIMENSION Z(2),AZ(2)
      COMMON/INTEG/JS4,JS,JE,ND
      T1=PI*DT
      IF(T.EQ.0.0) GO TO 18
      XPR=T/T1
      IPRI=NINT(XPR)
      IF(IPRI.EQ.0) GO TO 19
      XPRI=FLOAT(IPRI)
      XR=XPRI/XPR
      IF(ABS(XR-1.).LT.1.E-7) GO TO 18
      GO TO 19
   18 CONTINUE
      IF(JS4.NE.0.OR.JS.NE.0) GO TO 19
      ERROR=AZ(1)-Z(1)
      WRITE(2,1)T,AZ(1),Z(1),ERROR
    1 FORMAT(4(F10.7))
   19 CONTINUE
      RETURN
      END
C**** NUMERICAL MODULE
      SUBROUTINE DYMOD(TIME,DT,IOD)
      COMMON/INTEG/JS4,JS,JE,ND
      COMMON/MODEL/Z(2),AZ(2),DZ(2),A,B
      IPASS=0
    1 CONTINUE
C**** DERIVATIVE SECTION
      DZ(1)=Z(2)
      DZ(2)=-Z(1)
C**** INTEGRATION SECTION
      STP=TIME
      DO 2 INTCAL=1,ND
      TIME=STP
      CALL INTJS(JS4,JS,JE,IOD,IPASS)
      CALL SDINT(Z(INTCAL),DZ(INTCAL),TIME,DT,IOD,INTCAL)
    2 CONTINUE
C**** UPDATE INTEGRATION PASS NUMBER
      IPASS=IPASS+1
C**** CHECK FOR THE END OF THE STEP
      CALL INTPAS(IPASS,IOD)
      IF(JS.NE.0.OR.JS4.NE.0)      GO TO 1
      RETURN
      END
C**** ANALYTICAL MODULE
      SUBROUTINE ANMOD(TIME,ND)
      COMMON/MODEL/Z(2),AZ(2),DZ(2),A,B
      AZ(1)=SIN(TIME)
      RETURN
      END
```

```
C**** SUBROUTINE CONTROLLING THE INTEGRATOR PASSES
      SUBROUTINE INTJS(JS4,JS,JE,IOD,IPASS)
      IF(IOD.EQ.1) RETURN
      IF(IOD.EQ.2) JS=IPASS
      IF(IOD.EQ.4)JS4=IPASS
      RETURN
      END
C**** SUBROUTINE FOR CHECKING THE STEP COMPLETION
      SUBROUTINE INTPAS(IPASS,IOD)
      COMMON/INTEG/JS4,JS,JE,ND
      IF(IOD.EQ.1)                                  RETURN
      IF(JS.GT.2 )                                  JS=0
      IF(JS4.GT.4)                                  JS4=0
      IF(IOD.EQ.2.AND.IPASS.GT.2)                   IPASS=0
      IF(IOD.EQ.4.AND.IPASS.GT.4)                   IPASS=0
      RETURN
      END



C**** INTEGRATOR
      SUBROUTINE SDINT(XX,DX,TD,DTD,IOD,INTCAL)
      COMMON/INTEG/JS4,JS,JE,ND
      DIMENSION XA(2),DXA(2)
      IO=IOD
      IF(INTCAL.EQ.1) JN=0
      GO TO (6,5,1,1) , IO
    6 CONTINUE
      GO TO 7
C**************************************
    5 JS=JS+1
      IF(JS.EQ.3) GO TO 20
      IF(JS.EQ.2)  GO TO 10
C**************************************
    7 DT=DTD
    3 TD=TD+DT
      GO TO 10
    1 JS4=JS4+1
      IF(JS4.EQ.1) TJ0=TD
      IF(JS4.EQ.2) TJ1=TD
      IF(JS4.EQ.3) TJ2=TD
      IF(JS4.EQ.4) TJ3=TD
      IF(JS4.EQ.5) GO TO 30
      IF(JS4.EQ.1) GO TO 2
      IF(JS4.EQ.3) GO TO 4
      GO TO 10
    2 IF(JS4.EQ.1) H1=DT
      DT=DTD/2.
      GO TO 3
    4 TD=TD+DT
      IF(JS4.EQ.3) H3=DT
      DT=2.*DT
   10 CONTINUE
      IF(JS4.EQ.2) H2=DT
      IF(JS4.EQ.4) H4=DT
```

```
C**** INTEGRATE

      JN=JN+1
      IF(JN.GT.ND) JN=JN-ND
      GO TO (19,18,13,13), IO
C*********** **********
   19 XX=XX+DX*DT
      TD=TD-DTD
      RETURN
C**********  **********
   18 GO TO (11,12), JS
C********** **********
   11 DXA(JN)=DX
      XX=XX+DX*DT
      RETURN
C********** **********
   12 XX=XX+(DX-DXA(JN))*DT/2.0
      RETURN
C********** **********
   13 GO TO (14,15,16,17), JS4
C********** **********
   14 XA(JN)=XX
      DXA(JN)=DX
      XX=XX+DX*DT
      IF(INTCAL.NE.ND) TD=TJ0
      IF(INTCAL.NE.ND) DT=H1
      RETURN
C********** **********
   15 DXA(JN)=DXA(JN)+2.0*DX
      XX=XA(JN)+DX*DT
      IF(INTCAL.NE.ND) TD=TJ1
      IF(INTCAL.NE.ND) DT=H2
      RETURN
C********** **********
   16 DXA(JN)=DXA(JN)+2.0*DX
      XX=XA(JN)+DT*DX
      IF(INTCAL.NE.ND) TD=TJ2
      IF(INTCAL.NE.ND) DT=H3
      RETURN
C********** **********
   17 DXA(JN)=(DXA(JN)+DX)/6.0
      XX=XA(JN)+DXA(JN)*DT
      IF(INTCAL.NE.ND) TD=TJ3
      IF(INTCAL.NE.ND) DT=H4
      RETURN
C********** **********
   20 CONTINUE
      TD=TD-DTD
      RETURN
C********** **********
   30 CONTINUE
      TD=TD-DTD
      RETURN
      END
```

```
 Z =NUMERICAL  SOLUTIONS
AZ =ANALYTICAL SOLUTIONS
IOD =1
 DT =.01
 PI =10.
ENDT =.5
```

TIME	AZ	Z	ERROR
****	**	*	*****
0.0000000	0.0000000	0.0000000	0.0000000
0.1000000	0.0898785	0.0998800	-0.0100015
0.2000000	0.1888589	0.1988615	-0.0100027
0.3000000	0.2859522	0.2959542	-0.0100020
0.4000000	0.3801884	0.3901856	-0.0099972
0.5000000	0.4706259	0.4806109	-0.0099850

```
IOD=2
 DT=.01
 PI=10.
ENDT=.5
```

TIME	AZ	Z	ERROR
****	**	*	*****
0.0000000	0.0000000	0.0000000	0.0000000
0.1000000	0.0898785	0.0998351	-0.0099565
0.2000000	0.1888589	0.1986726	-0.0098137
0.3000000	0.2859522	0.2955250	-0.0095728
0.4000000	0.3801884	0.3894245	-0.0092361
0.5000000	0.4706259	0.4794329	-0.0088070

```
IOD =4
 DT =.01
 PI =10.
ENDT =.5
```

TIME	AZ	Z	ERROR
****	**	*	*****
0.0000000	0.0000000	0.0000000	0.0000000
0.1000000	0.0898785	0.0998334	-0.0099549
0.2000000	0.1888589	0.1986693	-0.0098104
0.3000000	0.2859522	0.2955202	-0.0095680
0.4000000	0.3801884	0.3894183	-0.0092299
0.5000000	0.4706259	0.4794255	-0.0087997

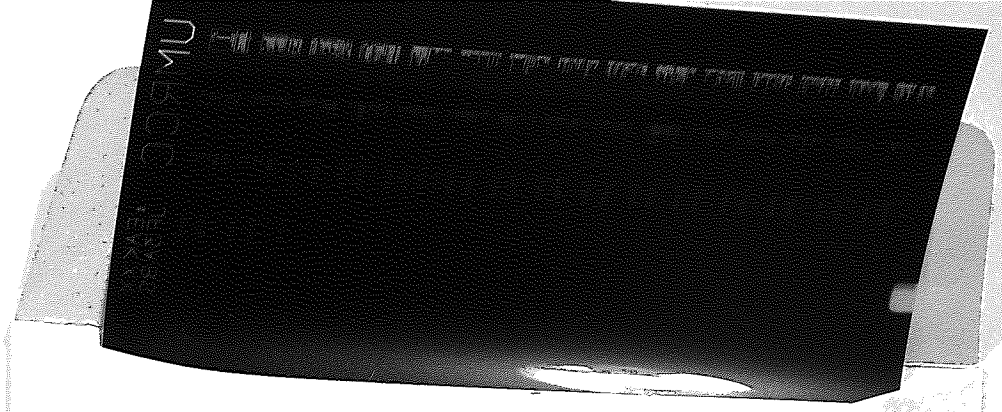
IOD = Integration order
DT = Step length
PI = Print interval
ENDT = End time
Z = Numerical solution
AZ = Analytical solution

Table B.1 : Results of the simulation of a second order system using the SDINT subroutine

B.1.1 Listings of the Simulators

The Contents of the Microfiche

Frame A1		: the contents
Frames A1,B1, ... O1		: listings of simulator II
	A2,B2, ...O2	which uses the comprehensive
	A3	column model (model II,
		chapter IV)



B.2 PREDICTION OF PHYSICAL PROEPRTIES

B.2.1 THE CRITICAL TEMPERATURES

The critical temperature T_c of organic compounds may be accurately estimated to within 1.0 percent by summing the additive contributions of Edjule (1,118). The sum of the contributions $\Sigma\Delta_T$ is then substituted into

$$T_c = \frac{100*T_b}{\Sigma\Delta_T}$$

where T_b and T_c are the boiling point and critical temperature in ^oK. respectively.

B.2.2 THE CRITICAL PRESSURES

The critical pressure of the organic compounds can also be estimated by summing the additive contributions of Edjule (1,114). Here we have

$$P_c = \frac{10^4*M}{(\Sigma\Delta_p)^2}$$

where M = the molecular weight g.mol.

P_c = the critical pressure atm.

$\Sigma\Delta_p$ = the sum of the additive contributions

B.2.3 THE CRITICAL COMPRESSIBILITY FACTORS

The critical compressibility may be estimated from the equation suggested by Edmister (1,120).

$$Z_c = 0.371 - \frac{0.0343 \log P_c}{(T_c/T_b - 1)}$$

where the symbols and their units are as defined before.

B.2.4 THE CRITICAL VOLUMES

The critical volume can be obtained from

$$V_c = \frac{Z_c R T_c}{P_c}$$

B.2.5 THE LIQUID DENSITIES

Having estimated the critical properties, the liquid densities can be estimated to an accuracy of 2 percent from the equation suggested by Goyal(1,121).

$$\zeta_\ell = \frac{P_c M}{T_c} \left(\frac{0.0653}{Z_c^{0.733}} - .09 T_r \right)$$

where ζ_ℓ = the liquid density g/cc.

T_c = the critical temperature ^oK.

P_c = the critical pressure atm.

T_r = the reduced temperature

B.2.6 THE LIQUID VISCOSITIES

The liquid viscosities can be estimated from the modified Arrhenius' relation (122)

$$\mu_b = 0.324 \zeta_{\ell b}^{0.5}$$

where $\zeta_{\ell b}$ = the density at boiling point g/cc.

$\mu_{\ell b}$ = the viscosity at boilint point centipoise

It must be noted that this equation is only applicable at the boiling point.

B.2.7 THE DIFFUSIVITY IN LIQUIDS

The theory of diffusion in liquids is less well developed than for gases. Diffusion coefficients in

liquids are typically about for orders of magnitude smaller than in gases. A recommended relation for estimation of diffusivities of non-electrolytes in liquids is due to Wilke and Chang (123) and is as follows:

$$\frac{D_{LV}}{T} = 7.4 * 10^{-8} * \frac{(XM)^{.5}}{(V_b)^{.6}}$$

In thermodynamically non-ideal solutions the effect concentration on D_L may be estimated by the equation suggested by Wilke (124)

$$\left(\frac{D_{LV}}{T}\right)_1 = \frac{d\ln a_1}{d\ln x_1} \left\{x_1 \left(\frac{D_{LV}}{T}\right)^{o}_2 + (1-x_1)\left(\frac{D_{LV}}{T}\right)^{o}_1\right\}$$

where

$\left(\frac{D_{LV}}{T}\right)_1$ = Stoke-Einstein group for diffusion of component 1 in 2 at concentration x_1

$\left(\frac{D_{LV}}{T}\right)^{o}_1$ = Stoke-Einstein group for diffusion of component 1 in 2 at infinite dilution of 1

$\left(\frac{D_{LV}}{T}\right)^{o}_2$ = Stoke-Einstein group for diffusion of component 2 in 1 at infinite dilution of 2

x_1 = mole fraction of 1

a_1 = activity of 1

D_L = diffusivity $cm^2./sec.$

v = viscosity centipoise

X = association parameter

The term $\frac{d\ln a_1}{d\ln x_1}$ may be determined from vapour-liquid equilibrium data and is 1.0 for ideal solutions. For non-ideal solutions, the term approaches 1.0 as x_1 approaches 1.

B.2.8 THE VAPOUR DENSITIES

The vapour densities or molar volumes may be calculated from the equations

$$V = \frac{ZRT}{P}$$

$$\zeta_v = \frac{1}{v}$$

where the compressibility factor may be obtained from the Nelson-Obert charts (1).

B.2.9 THE VAPOUR VISCOSITIES

The Bromley and Wilke (125) modification of the theoretical Hischfelden method (126) for computing the viscosities of low pressure pure vapours is known to give good results. It requires the knowledge of the critical volume of the vapour which can be predicted and is of the form

$$\nu^o = \frac{33.3(MT_c)^{.5}}{V_c^{2/3}} \{f(1.33T_r)\}$$

and $$f(1.33T_r) = 1.058T_r^{0.645} - \frac{0.261}{(1.9T_r)^{0.9\log(1.9T_r)}}$$

where

ν^o	= the viscosity	micropoise
T_c	= the critical temperature	$^oK.$
V_c	= the critical volume	cc./g.mole
T_r	= the reduced temperature	

B.2.10 THE DIFFUSIVITY IN VAPOURS

The study of diffusion, along with viscosity and thermal conduction in vapours and gases, is a part of the well-developed kinetic theory of gases. One of the accounts of this theory is that of Hirschfelder, Curtiss and Bird (126), who gave equations based on various assumptions regarding the nature of the interaction between molecules at collision, from which the values of the diffusion coefficient for a binary mixture may be calculated. The most advanced treatment predicts that the diffusion coefficient should vary only slightly with composition, and this is confirmed by experiment.

When experimentally determined diffusivities are not available, several prediction methods based on the kinetic theory are available to provide estimates. When accurate estimates are desired the Wilke and Lee modification (126) of the equation by Hirschfelder, Bird and Spotz (127) is recommended

$$D_G = \frac{BT^{3/2} \sqrt{(1/M_1) + (1/M_2)}}{Pr_{12}^2 I_D}$$

where

D_G	= the diffusivity	$cm.^2/sec.$
T	= absolute temperature	$^oK.$
M_1, M_2	= molecular weights of components 1 and 2	g.mole
r_{12}	= collision diameter	Angstroms
	$= \frac{(r_o)_1 + (r_o)_2}{2}$	

r_o = $(1.18V_b)^{1/3}$

V_b = molal volume of the liquid cc./g.mol. at normal boiling point

I_D = Collision integral for diffusion function KT/e_{12}

$\frac{e_{12}}{K}$ = $\sqrt{(\frac{e_1}{K})(\frac{e_2}{K})}$

K = Boltzman constant = 1.38×10^{-6} erg/^oK.

$\frac{e}{K}$ = $1.15T_b$

The collision integral can be calculated from

$$I_D = \frac{L}{(T^*)^M} + \frac{N}{Exp(RT^*)} + \frac{Z}{Exp(WT^*)}$$

where

L = 1.16415; M = .14874 N = .52487

R = .77320; Z = 2.16178; W = 2.43787

$T^* = \frac{KT}{e}$

Also $B = (1.0 - 2.46\sqrt{(1/M_1 + 1/M_2)}) \times 10^{-4}$

For multicomponent systems, the diffusivity may be a strong function of composition and is different for each component (124).

B.2.11 THE DENSITIES OF THE LIQUID AND VAPOUR MIXTURES

The fictitious or average density for binary liquid mixtures is defined as follows:

$$\zeta_{m\ell} = (x\zeta_\ell)_1 + (x\zeta_\ell)_2$$

similarly for the vapour phase

$$\zeta_{mv} = (y\zeta_v)_1 + (y\zeta_v)_2$$

where x and y are the mole fractions in liquid and vapour phases.

B.2.12 THE VISCOSITIES OF THE LIQUID AND VAPOUR MIXTURES

The viscosity of a vapour mixture may be calculated from

$$\nu_{mv} = \frac{\Sigma y_i \nu_i (M_i)^{0.5}}{\Sigma \; y_i (M_i)^{0.5}}$$

where

ν_{mv} = the viscosity of the vapour mixture

ν_i = the component viscosities

M_i = the component molecular weights

The viscosity of a binary liquid mixture can be calculated from

$$\nu_{m\ell} = ((x\nu)_1^{1/3} + (x\nu)_2^{1/3})^3$$

where x refers to the mole fractions and subscripts 1 and 2 refer to the components.

B.2.13 THE SPECIFIC HEAT CAPACITIES

The low-pressure heat capacities of pure organic compounds may be estimated with good accuracy with Dobratz's equation (114,130)

$$C_p^o = 4R + n_r' \frac{R}{2} + \Sigma q_i C_{vi} + \frac{3n-6-n_r'-\Sigma q_{iv}}{\Sigma q_i} \Sigma q_i C_{\delta i}$$

in conjunction with the tables given by Reid and Sherwood (1,114,130) which give the Meghreblian's recommendations (132) for the characteristic stretching and bending vibrational wave numbers (v and δ), along

with the corresponding constants of the heat-capacity equation

$$C_p^o = A + BT + CT^2$$

as obtained from the analysis of Crawford and Parr (133).

In these equations

C_p = the specific heat capacity cal./(g.mole)($^oK.$)

R = the universal gas constant cal./(g.mole)($^oK.$)
= 1.987

n = the total number of atoms in the molecule

q_i = the number of atoms of the ith type

Σq_i = the total number of bonds in the molecule

C_{vi} and $C_{\delta i}$ = the Einstein functions for bonds of the ith type

n_r' = the number of single bonds about which internal rotation of groups can take place

A P P E N D I X C

C.1 THE PROPERTIES OF THE LIQUID SYSTEM

C.1.1 VAPOUR-LIQUID EQUILIBRIUM DATA

The vapour-liquid equilibrium of the binary liquid system consisting of Trichloroethylene and Tetrachloroethylene at atmospheric pressure has been investigated by Bachman (135). The activity coefficients needed for the calculation of Van-Larr constants are also given in the aforementioned article.

C.1.2 VAPOUR-PRESSURE-TEMPERATURE DATA

The vapour-pressure-temperature data needed for the calculation of Antoine equation constants are found in The International-Critical-Tables (138).

C.1.3 MISCELLANEOUS PROPERTIES AT 20°C

Property	Trichloroethylene	Tetrachloroethylene	Units
ζ	1.4642	1.6475	g./cc.
$\bar{C}_p$	0.9040	0.8830	J./g.°C
λ	239.60	209.50	J./g.

where: ζ = density

$\bar{C}_p$ = specific heat capacity

λ = latent heat of vapourization

The data given in the table above are from the International Critical Tables (138).

C.1.3 THE CRITICAL PROPERTIES

The critical properties of the two components of the liquid system are shown in the table below.

Property	Trichloroethylene	Tetrachloroethylene	Units
P_c	54.448	40.72	atm.(abs.)
T_c	560.94	597.80	$^oK.$
V_c	2.68×10^{-4}	3.44×10^{-4}	$m^3/mol.$
Z_c	0.265	0.286	-

where: P_c = critical pressure

T_c = critical temperature

Z_c = critical compressibility

V_c = critical volume

C.1.4 MISCELLANEOUS PROPERTIES AT BOILING POINTS

Property	Trichloroethylene	Tetrachloroethylene	Units
ζ_{lb}	10089.734	8686.75	$mol./m^3$
V_b	2.95×10^{-2}	3.21×10^{-2}	$m^3./mol.$

where: ζ_{lb} = liquid density at boiling point

V_b = molar volume at boiling point

C.2 THE ESTIMATION OF THE HEAT LOSSES

C.2.1 HEAT LOSSES FROM THE PIPE SECTION WHICH ENABLES GRAVITY FLOW

The heat losses from the pipe section, added to the top of the column in order to enable gravity flow, will cause the condensation of the overhead vapour passing through the pipe which, in turn, appears in the form of additional reflux and thus affects the operation of the column.

The following assumptions have to be made to render the estimation of the heat thus lost to the atmosphere possible:

(i) the resistance to heat transfer is mainly due to the fibre glass lagging

(ii) the glass is at the same temperature as the overhead vapour at steady-state

Typical Estimation Procedure for Steady-State Experiment No.5

The thermal conductivity of the lagging	= 0.27 B.T.U./hr.^{o}F.ft^{2}./in.	
Total heat transfer area	= 2.57	ft.^{2}
Atmospheric temperature	= 66.2	^{o}F.
Glass Temperature	= 188.6	^{o}F.
The thickness of the lagging	= 1	inch

$$\therefore \quad Q = \frac{KA\delta T}{x} = \frac{(0.27)(2.5687)(188.6-66.2)}{1}$$

$$= 84.9 \quad \text{B.T.U./hr.}$$

$$= 89.6 \quad \text{kJ./hr.}$$

Therefore the measured reflux rate must be corrected as follows:

Measured reflux rate = 118.5 cc./min.

= 61.2 g.mol./hr.

Additional reflux = $\frac{89.568}{31.5074}$ = 2.8 g.mol./hr.

$\therefore$ Total reflux = 82.0 g.mol./hr.

C.2.2 HEAT LOSSES FROM THE COLUMN

The heat losses from the column will simply appear as the extra heat which has to be provided by the reboiler in addition to the heat needed to vapourize one mole of the liquid inside the reboiler. The assumptions made are the same as the ones made in order to estimate the amount of heat losses from the gravity flow pipe section. Average temperatures are assumed in the enriching and stripping sections.

Typical Estimation Procedure for Steady-State Experiment No.5

(a) The Enriching Section

Average Vapour Temperature = 200.5 ^{o}F.

Area = 1.68 ft.^{2}

Ambient Temperature = 66.2 ^{o}F.

$$\therefore \quad Q_e = \frac{K\ A_e\ \delta T_e}{x}$$

$$= \frac{(0.27)\,(1.67836)\,(200.468-66.2)}{1} = 60 \text{ B.T.U./hr.}$$

$$= 64.2 \text{ kJ./hr.}$$

(b) The Stripping Section

Average Temperature = 225.8 ^{o}F.

Area = 1.4 ft.^{2}

Ambeint Temperature = 66.2 ^{o}F.

$$\therefore Q_s = \frac{k\ A_s\ \delta T_s}{x}$$

$$= \frac{(0.27)\,(1.40216)\,(225.804-66.2)}{1} \simeq 61.2 \text{ B.T.U./hr.}$$

$$\simeq 64.6 \text{ kJ./hr.}$$

(c) The Heat Losses from the Reboiler

Assuming that the reboiler is spherical the estimated uncovered area is approximately 0.089 square metres. Now

$$Q_b = UA\ \delta T_b$$

$$= 30 \times 0.0894 \times (114-19) \times 4.186 \simeq 1066 \text{ kJ./hr.}$$

Therefore an estimate of the total heat losses can be obtained by summing the individual estimates of heat losses calculated in sections (a), (b) and (c) as

$$\delta Q_{lost} = 64.2 + 64.6 + 1066 \simeq 1195 \text{ kJ./hr.}$$

Actual heat input $Q_{actual} \simeq 4805$ kJ./hr.

$$\therefore \quad Q_{adiabatic} \simeq 3610 \text{ kJ./hr.}$$

A P P E N D I X D

CONTENTS

D.1 Description of the latest version of the HADIOS Executive and its modifications for this research

D.2 The listing of the HADIOS Executive in the Assembler symbolic language

D.3 The listing of subroutine 5; modification No.1

D.4 The listing of the patch added to the analogue inputs : modification No.2

This version of the HADIOS Executive Package provides facilities for accessing all the available HADIOS devices from a BASIC program. It therefore supersedes all previous versions.

Devices Available

(1) Analogue inputs

48 analogue channels (numbered 0-47) are multiplexed through a common ADC which has an input range of 0-5V. The converted digital input to the computer is in the range 0-1023.

(2) Counter inputs

Three counters are available. Each counter has a range 0-255 and after 255 pulses have been counted the counter returns to zero and resumes counting. The counters can also be programmed to interrupt on reaching a count of 127. In both cases the counters can be preset to an initial (positive) value $\leq$255 after each scan or counter interrupt.

(3) Digital inputs

Two digital inputs are available. Each has 16 parallel input lines whose values (0 or 1) can be read into the computer.

(4) Digital outputs

Two digital outputs are available. Each has 16 parallel output lines whose values (0 or 1) can be sent out by the computer. The values output remain constant until the next 16 bit word is

sent out. Four forms of output are available (see below).

Programming Details

All HADIOS input/output is done when subroutine 1 (see below) is first called and thereafter at the end of a time interval selected by the user.

The user communicates with HADIOS by CALL's from his BASIC program as follows:

CALL (1, A(0), B(0))

Subroutine 1 is the basic scanning routine. Arrays A (dimensioned 13) and B (dimensioned 120) contain the users parameters and variables.

A(0)		Scanning interval (sec)
A(1)		Devices required
	=1	Analogue inputs
	=2	Counter 1
	=4	Counter 2
	=8	Counter 3
	=16	Digital input A
	=32	Digital input B
	=64	Digital output A
	=128	Digital output B

The required set of devices is selected by setting A(1) equal to the sum of the appropriate values above.

A(2) Number of scans required (including the initial scan at time zero).

A(3) First analogue channel.

A(4) Last analogue channel.

A(5) Number of samples of each analogue channel per scan (ensemble number).

A(6) Counter 1 scan type.

=0 no counter interrupt.

=1 enable counter interrupt.

A(7) Counter 1 preset value.

A(8) Counter 2 scan type.

A(9) Counter 2 preset value.

A(10) Counter 3 scan type.

A(11) Counter 3 preset value.

A(12) Digital output A mode.

=0 from 16 element array at BASIC level (see below).

=1 from subroutine 3 or 4 (see below).

=2 from user supplied subroutine (see below).

A(13) Digital output B mode.

B(0) - B(47) Analogue input channel readings (each averaged over A(5) samples).

B(48) Counter 1 interrupt time (sec).

B(49) Counter 1 contents at scanning time.

B(50) Number of interrupts by counter 1 during last scanning interval.

B(51) Counter 2 interrupt time (sec).

B(52) Counter 2 contents at scanning time.

B(53) Number of interrupts by counter 2 during last scanning interval.

B(54) Counter 3 interrupt time (sec).

B(55) Number of interrupts by counter 3 during last scanning interval.

B(57) - B(72) Values (0 or 1) read on bits 1-16 of digital input A.

B(73) - B(88) Values (0 or 1) read on bits 1-16 of digital input B

B(89) - B(104) Values (0 or 1) output on bits 1-16 of digital output A (when A(12)=0).

B(105) - B(120) Values (0 or 1) output on bits 1-16 of digital output B (when A(13)=0).

CALL (2)

This CALL causes the program to wait for the next clock interrupt (scan time) if all scans requested (A(2)) have not been done. Otherwise the BASIC program continues from after the CALL (2).

On a clock interrupt, a scan is performed and the BASIC program continues from after the previous CALL (1, ...) - the inter-scan processing section of the program.

CALL (2) disenables clock and counter(s) interrupt when all scans requested have been done.

CALL (3, D, N, X)

This subroutine provides for a special form of digital output to send out an analogue signal by means of extra hardware when A(12) = 1 or A(13) = 1.

D =O digital output A.

=1 digital output B.

N = analogue output channel (1-15).

X = digital equivalent of analogue output. For O < X < 32767, the analogue output will be O-10v.

CALL (4, D, I, C)

This subroutine controls the format of the digital output when A(12) = 1 or A(13) = 1 as follows:

D =O digital output A.

=1 digital output B.

I <O reset all 16 bits to zero.

>O set bits 15-2*I and 16-2*I to value of C leaving other bits unchanged, O < 1 < 7.

C = O, 1, 2 or 3 only.

This subroutine has been provided to control up to 8 valve drives. Normally, therefore, only 3 values of C will be used (say O, 1 and 2).

Sense Switch Usage

S.S. 1 - Normal use for terminating a BASIC program (not recommended).

S.S. 2 - As for S.S. 1 but interrupts are also disenabled (see below).

S.S. 3 - INPUT statement reads data from tape.

S.S. 4 - PRINT statement writes data to tape.

Error Messages

Error Message Format : ERROR XY LINE NNN, where XY is one of the following:

1. TF - the clock interrupt frequency is too small and so BASIC code was still being excecuted when a clock interrupt took place. This would obviously lead to a backlog of processing at the BASIC level if it were allowed to go unchecked and so execution is terminated.

2. NR - an unidentifiable interrupt has occurred and execution is terminated.

3. NC - the Hadios controller has interrupted the central processor but the interrupting device was not a counter. Execution is terminated.

4. UI - the execution of the program has been terminated by user interference. This is caused by setting sense switch 2. When interrupt is occurring it is preferable to terminate execution in this way rather than by setting sense switch 1 as the setting of sense switch 2 causes all interrupts to be disenabled.

5. RI - a real to integer conversion error has occurred in the HADIOS EXECUTIVE i.e. conversion of a real number outside the range -32768 to +32767 was attempted.

6. SE - user supplied subroutine has been called (A(12) or A(13) = 2) but is not loaded.

User Supplied Subroutine

The user may also supply his own DAP-16 routine to control a digital output device.

The present package contains a dummy version of this routine (called MYSR) which does not cause any

output. The user supplied subroutine is called by setting A(12) or A(13) = 2. The starting address of the routine should be patched into location '37603 (SPSR).

Note that only one of subroutine 3, 4 or the special routine may be used for digital output A or B in the same program and at present only one user supplied routine may be added to the package.

In all cases the requested digital output will be performed at the next clock interrupt.

Further Subroutines

Additional routines may be added to the HADIOS Executive (e.g. for graphics etc). Such routines must be loaded in sector 35 and below with the base of COMMON (if any) at '35777. There can be 6 routines called from BASIC (numbered 5 to 10). The starting addresses of the routines should be patched into locations '522 onwards and '230 (DAC IBUF) should be patched into '36221 onwards for as many subroutines as can be called from BASIC (i.e. '36221 for subroutine 5 etc).

The address of the first location below the subroutines should be patched into location '7367.

Note that only locations '733 - '777 are available for BASE in sector 0. If more BASE is required it must be located elsewhere (by setting the B register at load time etc).

Counter Calculations

The counter rate may be calculated either from the counter interrupt time or from the number of interrupts

over a scan interval and the counter contents at the next scan. Thus for counter 1

Rate = (127 - A(7))/B(48)

or Rate = ((127 - A(7))*B(50) + B(49))/A(0)

with similar expressions for counters 2 and 3.

The latter form is more accurate if the rate is constant over the period A(0) but the former gives an 'instantaneous' rate.

Note that the values of B(48), B(51) and B(54) have no significance at time zero (first scan).

Executive Package Revision 02 (1978)

Modification No. 01

Use of subroutine 3 allows only one analogue channel per digital output to be changed at a clock interrupt.

It may be that more than one analogue output is to be changed and that the changes need not wait until the next clock interrupt.

Subroutine 5 has been added to implement this facility. In CALL (5, D, N, X) the arguments have the same meaning as in subroutine 3 but the value X is output immediately on channel N of device D.

Note that if digital output is only through subroutine 5, A(1) should not be set for the digital output device.

Digital output at a clock interrupt may still be carried out by all modes previously described.

Subroutine 5 has been loaded from '35734. Further subroutines (6-10) may be added below this address.

Executive Package Revision 02 (1979)

Modification No. 02

This patch enables the scanning interval to be divided into as many subintervals of 20 μsec duration as possible - a value of A(5) is calculated. The samples of the analogue input channels are thus spaced out over the entire scanning interval as opposed to being taken instantaneously according to a prespecified value of A(5).

The sole advantage of this modification is that it enables the noise (if any) to be smoothed out more effectively during the scanning of the analogue input channels.

Note that A(5) no longer needs to be specified. Also CTS, location '37776 contains a big negative number which can be keyed in at load time. The bigger the number the smaller the number of samples. The present value is -33.

```
0001                                *HADIOS EXECUTIVE  1978/1
0002                                *         REV 02
0003                                *
0004                                      REL
0005                                      ENT   HADIOS,SKST
0006                                      ENT   IFLG
0007                                      ENT   ERCL
0008                                      SETB  BAS1
0009                 000070       DATA  EQU   '70
0010                 000170       ANAG  EQU   '170
0011                 000470       CTR1  EQU   '470
0012                 000570       SET1  EQU   '570
0013                 000670       CTR2  EQU   '670
0014                 000770       SET2  EQU   '770
0015                 000270       CTR3  EQU   '270
0016                 000370       SET3  EQU   '370
0017                 001170       DGIA  EQU   '1170
0018                 001070       DGIB  EQU   '1070
0019                 001370       DGOA  EQU   '1370
0020                 001270       DGOB  EQU   '1270
0021                 001770       HAD   EQU   '1770
0022                 000020       CLK   EQU   '20
0023                 000220       SCLK  EQU   '220
0024                 000034       SIF   EQU   '34
0025                 000037       SBF   EQU   '37
0026                 000230       IBUF  EQU   '230
0027                 000515       CJST  EQU   '515
0028                 004064       SS    EQU   '4064
0029                 000675       C12   EQU   '675
0030                 000676       C21   EQU   '676
0031                 000653       L22   EQU   '653
0032                 000654       H22   EQU   '654
0033                 000670       D22   EQU   '670
0034                 000674       M22   EQU   '674
0035                                *
0036                                * INTERRUPT ENTRY POINT
0037                                *
0038 000000          0 000000     SKST  DAC   **
0039 000001          34 0020            SKS   CLK
0040 000002          0 01 000017        JMP   LNKA
0041 000003          34 1770            SKS   HAD
0042 000004          0 01 000007        JMP   CONT
0043 000005          0 10 01606         JST   ERCL                NOT RECOGNISED
0044 000006          147322             HCI   1,NE
0045                                *
0046                                * HADIOS INTERRUPTING
0047                                *
0048 000007          34 0470      CONT  SKS   CTR1
0049 000010          0 01 000032        JMP   LNKB
0050 000011          34 0670            SKS   CTR2
0051 000012          0 01 000045        JMP   LNKC
0052 000013          34 0270            SKS   CTR3
0053 000014          0 01 000060        JMP   LNKD
0054 000015          0 10 01606         JST   ERCL                NOT COUNTER
0055 000016          147303             BCI   1,NC
0056                                *
0057                                * CLOCK INTERRUPT LINK
```

```
0058                            *
0059                            *
0060                            *       LINK    LNKA,1,LNKA
0061 0017    0 10 0073  LNKA    JST     CIH
0062 0020    0000001            BSZ     5
0063 0025    0000001            OCT     1
0064 0026    0 0000026          DAC     LNKA+1
0065 0027    0 0000000  LNKA    DAC     **
0066 0030    0 35 0026          LDX     *-2
0067 0031    0 01 0120          JMP     CIH
0068                            *
0069                            * COUNTER INTERRUPT LINKS
0070                            *
0071                            *
0072                            *       LINK    LNKB,10,LNKB
0073 0032    0 10 0073  LNKB    JST     CIH
0074 0033    0000010            BSZ     5
0075 0034    0000010            OCT     10
0076 0035    0 0000033          DAC     LNKB+1
0077 0036    0 0000000  LNKB    DAC     **
0078 0037    0 35 0035          LDX     *-2
0079 0040    0 01 0120          JMP     CIH
0080                            *
0081                            *       LINK    LNKC,10,LNKC
0082 0041    0 10 0073  LNKC    JST     CIH
0083 0042    0000010            BSZ     5
0084 0043    0000010            OCT     10
0085 0044    0 0000046          DAC     LNKC+1
0086 0045    0 0000000  LNKC    DAC     **
0087 0046    0 35 0044          LDX     *-2
0088 0047    0 01 0120          JMP     CIH
0089                            *
0090                            *       LINK    LNKD,10,LNKD
0091 0050    0 10 0073  LNKD    JST     CIH
0092 0051    0000010            BSZ     5
0093 0052    0000010            OCT     10
0094 0053    0 0000057          DAC     LNKD+1
0095 0054    0 0000000  LNKD    DAC     **
0096 0055    0 35 0053          LDX     *-2
0097 0056    0 01 0120          JMP     CIH
0098                            *
0099                            * COMMON INTERRUPT HANDLER
0100                            *
0101 0073    0 0000000  CIH     DAC     **
0102 0074   -0 15 0073           STX*    CIH
0103 0075    0 35 0073          LDX     CIH
0104 0076    1 13 0001          IMA     1,1
0105 0077    0000043            INK
0106 0100    0000005            SGL
0107 0101    1 04 0002          STA     2,1
0108 0102    0 02 0000          LDA     SKST
0109 0103    1 04 0004          STA     4,1
0110 0104    1 02 0005          LDA     5,1
0111 0105    1401401            CMA
0112 0106    0 03 0162          ANA     MASK
0113 0107    0 04 0162          STA     MASK
0114 0110    74 0020            SMK     '20
```

```
0115 00111    1 02 000007        LDA   7,1
0116 00112    0 04 00117         STA   CIHA
0117 00113    000201             IAB
0118 00114    1 04 000003        STA   3,1
0119 00115    000011             DXA
0120 00116   -0 01 00117         JMP*  CIHA
0121 00117    000000     CIHA BSZ   1
0122                     *
0123                     * COMMON INTERRUPT RETURN
0124                     *
0125 00120    1 02 000003 CIR   LDA   3,1
0126 00121    000201             IAB
0127 00122    1 02 000005        LDA   5,1
0128 00123    140401             CMA
0129 00124    001001             INR
0130 00125    0 03 00162         ANA   MASK
0131 00126    1 05 000005        ERA   5,1
0132 00127    0 04 00162         STA   MASK
0133 00130    74 0020            SMK   '20
0134 00131    1 02 000004        LDA   4,1
0135 00132    0 04 00160         STA   CIRA
0136 00133    1 02 000000        LDA   0,1
0137 00134    0 04 00161         STA   CIRX
0138 00135    1 02 000002        LDA   2,1
0139 00136    171020             OTK
0140 00137    1 13 000001        IMA   1,1
0141 00140    0 35 00161         LDX   CIRX
0142 00141    000001             ENB
0143 00142   -0 01 00160         JMP*  CIRA
0144                     *
0145                     * COMMON INTERRUPT INITIATOR
0146                     *
0147 00143    0 000000   CII   DAC   **
0148 00144   -0 35 00143        LDX*  CII
0149 00145    0 12 00143         ISZ   CII
0150 00146    1 02 000000        LDA   0,1
0151 00147    140401             CMA
0152 00150    0 03 00162         ANA   MASK
0153 00151    1 05 000000        ERA   0,1
0154 00152    74 0020            SMK   '20
0155 00153    0 04 00162         STA   MASK
0156 00154   -0 02 00143        LDA*  CII
0157 00155    0 12 00143         ISZ   CII
0158 00156    1 04 000002        STA   2,1
0159 00157   -0 01 00143         JMP*  CII
0160 00160    000000     CIRA BSZ   1
0161 00161    000000     CIRX BSZ   1
0162 00162    000000     MASK BSZ   1
0163 00163    005243     FHR  OCT   5243
0164                     *
0165                     *
0166                     * DISPATCHER
0167                     *
0167 00164    0 35 00674 DISP  LDX   =-5
0168 00165    1 02 00211         LDA   GOAD+5,1
0169 00166    100040             SZR
0170 00167    0 01 00177         JMP   DISC
0171 00170    100010             SKP
```

```
0172 00171    0 01 00175          JMP   STOP
0173 00172    0 12 00000          IRS   0
0174 00173    0 01 00165          JMP   DISP+1
0175 00174    0 01 00164          JMP   DISP
0176 00175    0 10 01606  STOP    JST   ERCL
0177 00176    152711              BCI   1,HI
0178 00177    0 04 00203  DISO    STA   DISS                USER INTERRUPED
0179 00200    140040              CRA
0180 00201    1 04 00211          STA   GOAD+5,1
0181 00202   -0 01 00203          JMP*  DISS
0182 00203    000000      DISS    BSZ   1
0183 00204    000000      GOAD    BSZ   5
0184                      *
0185                      * BASIC ENTRY POINT
0186                      *
0187 00211    0 02 00230  CALL    LDA   IBUF
0188 00212    0 07 00515          SUB   CJST
0189 00213    0 04 00000          STA   0
0190 00214   -1 01 00214          JMP*  TABL-1,1
0191 00215    0 000227    TABL    DAC   SUB1
0192 00216    0 000372            DAC   SUB2
0193 00217    0 000451            DAC   SUB3
0194 00220    0 000516            DAC   SUB4
0195 00221    0 004064            DAC   SS
0196 00222    0 004064            DAC   SS
0197 00223    0 004064            DAC   SS
0198 00224    0 004064            DAC   SS
0199 00225    0 004064            DAC   SS
0200 00226    0 004064            DAC   SS
0201                      *
0202                      * SUBROUTINE 1
0203                      *
0204                      *
0205                      *     SAVE  SIP1,SHP1
0206 00227                SUB1  BSS   0
0207 00227    0 02 00034          LDA   SIP
0208 00230    0 04 00442          STA   SIP1
0209 00231    0 02 00037          LDA   SHP
0210 00232    0 04 00443          STA   SHP1
0211 00233    0 02 00437          LDA   NEXT
0212 00234    0 04 00236          STA   **2
0213 00235    0 01 00237          JMP   **2
0214 00236    0 000000            DAC   **
0215 00237   -0 10 00441          JST*  FAT
0216 00240    000002              DEC   2
0217 00241    000000      PARS    BSZ   2
0218 00243   -0 10 00653          JST*  L22
0219 00244   -0 000241            LAC*  PARS
0220 00245   -0 10 00674          JST*  M22
0221 00246    0 000447            DAC   FSW
0222 00247   -0 10 00676          JST*  C21
0223 00250    0 01 00370          JMP   ERI
0224 00251    140407              TCA
0225 00252    0 04 00440          STA   CINT
0226 00253    0 02 00241          LDA   PARS
0227 00254    0 06 00673          ADD   =1W
0228 00255    0 04 01452          STA   REP+3
```

```
0229 00256    0 12 00241        IRS   PARS
0230 00257    0 12 00241        IRS   PARS
0231 00260    0 35 00672        LDX   =-13
0232 00261    0 15 00446        STX   KT
0233 00262   -0 10 00653        JST*  L22
0234 00263   -0 000241           DAC*  PARS
0235 00264   -0 10 00676        JST*  C21
0236 00265    0 01 00370        JMP   ERI
0237 00266    0 35 00446        LDX   KT
0238 00267    1 04 00435        STA   CTRS+13,I
0239 00270    0 12 00241        IRS   PARS
0240 00271    0 12 00241        IRS   PARS
0241 00272    0 12 000000       IRS   0
0242 00273    0 01 00261        JMP   *-10
0243 00274    0 02 00435        LDA   DACS
0244 00275    0 04 00063        STA   '63
0245 00276    0 02 00436        LDA   FRST
0246 00277    0 04 00061        STA   '61
0247 00300    0 35 00674        LDX   =-5
0248 00301    1400040           CLA
0249 00302    0 04 00515        STA   IFLG
0250 00303    0 04 00162        STA   MASK
0251 00304    0 04 01601        STA   SCAN
0252 00305    1 04 00211        STA   GOAD+5,I
0253 00306    0 12 000000       IRS   0
0254 00307    0 01 00305        JMP   *-2
0255                    *
0256                    *       INTI  LNKA,ACLK,CLK
0257 00310    0 10 00143        JST   CII
0258 00311    0 000025          DAC   LNKA-2
0259 00312    0 001060          DAC   ACLK
0260 00313    14 0020           OCP   CLK
0261
0262                    *
0263                    *       DVCE  =2,A1
0264 00314    0 02 00420        LDA   CTRS
0265 00315    0 03 00671        ANA   =2
0266 00316    100040            SNZ
0267 00317    0 01 00332        JMP   A1
0268
0269                    *
0270                    *       SET   6,SETI
0271 00320    0 02 00426        LDA   CTRS+6
0272 00321    74 0570           OTA   SETI
0273 00322    0 01 00321        JMP   *-1
0274
0275                    *
0276                    *       CTII  5,A1,LNKB,ICTI,CTRI
0277 00323    0 02 00425        LDA   CTRS+5
0278 00324    100040            SNZ
0279 00325    0 01 00332        JMP   A1
0280 00326    0 10 00143        JST   CII
0281 00327    0 000040          DAC   LNKB-2
0282 00330    0 000063          DAC   ICTI
0283 00331    14 0470           OCP   CTRI
0284
0285                    *
0286                    *       DVCE  =4,A2
0287 00332                      A1    BSS   0
0288 00332    0 02 00420        LDA   CTRS
0289 00333    0 03 00670        ANA   =4
```

```
0286 00334   101040          SNZ
0287 00335   0 01 00350      JMP   A2
0288                        *
0289                        *     SET   8,SET2
0290 00336   0 02 00430      LDA   CTRS+8
0291 00337   74 0770         OTA   SET2
0292 00340   0 01 00337      JMP   *-1
0293                        *
0294                        *     CTII  7,A2,LNRC,ICT2,CTR2
0295 00341   0 02 00427      LDA   CTRS+7
0296 00342   101040          SNZ
0297 00343   0 01 00350      JMP   A2
0298 00344   0 10 00143      JST   CII
0299 00345   0 000053        DAC   LNRC-2
0300 00346   0 000224        DAC   ICT2
0301 00347   14 0270         OCP   CTR2
0302                        *
0303                        *     DVCP  =8,INT
0304 00350                  A2    BSS   0
0305 00350   0 02 00420      LDA   CTRS
0306 00351   0 03 00267      ANA   =8
0307 00352   101040          SNZ
0308 00353   0 01 00366      JMP   INT
0309                        *
0310                        *     SET   10,SET3
0311 00354   0 02 00432      LDA   CTRS+10
0312 00355   74 0370         OTA   SET3
0313 00356   0 01 00355      JMP   *-1
0314                        *
0315                        *     CTII  9,INT,LNRD,ICT3,CTR3
0316 00357   0 02 00431      LDA   CTRS+9
0317 00360   101040          SNZ
0318 00361   0 01 00366      JMP   INT
0319 00362   0 10 00143      JST   CII
0320 00363   0 000044        DAC   LNRD-2
0321 00364   0 000245        DAC   ICT3
0322 00365   14 0270         OCP   CTR3
0323 00366   000401        INT   ENB
0324 00367   0 01 00164      JMP   DISP
0325 00370   0 10 01000     FRI   JST   FRCL
0326 00371   151311            RCI   1,RI
0327                        *
0328                        *  SUBROUTINE 2
0329                        *
0330 00372   000001        SUB2  INH
0331                        *
0332                        *     SAVE  SIP2,SBP2
0333 00373   0 02 00034      LDA   SIP
0334 00374   0 04 00444      STA   SIP2
0335 00375   0 02 00037      LDA   SBP
0336 00376   0 04 00445      STA   SBP2
0337 00377   140040          CRA
0338 00400   0 04 00515      STA   IFLG
0339 00401   0 02 01601      LDA   SCAN
0340 00402   0 07 00421      SUB   CTRS+1
0341 00403   101400          SMI
0342 00404   0 01 00407      JMP   *+3
```

REAL TO INTEGER

```
0343 000405     000401                  ENB
0344 000406     0 01 001E4              JMP     DISP
0345 000407     14 0220                 OCP     SCLK
0346 000410     14 0570                 OCP     SET1
0347 000411     14 0770                 OCP     SET2
0348 000412     14 0370                 OCP     SET3
0349                            *
0350                            *       RSET    SIP2,SBP2
0351 000413     0 02 000444             LDA     SIP2
0352 000414     0 04 000034             STA     SIP
0353 000415     0 02 000445             LDA     SBP2
0354 000416     0 04 000037             STA     SBP
0355 000417    -0 01 01E000             JMP*    CLRF
0356 000420     000000          CTRS    BSZ     13
0357 000435     0 000000        DACS    DAC     SKST
0358 000436     .177777         FRST    DEC     -1
0359 000437     0 000231        NEXT    DAC     IBUF+1
0360 000440     000000          CINT    BSZ     1
0361 000441     0 000000        FAT     XAC     FSAT
0362 000442     000000          SIP1    BSZ     1
0363 000443     000000          SBP1    BSZ     1
0364 000444     000000          SIP2    BSZ     1
0365 000445     000000          SBP2    BSZ     1
0366 000446     000000          KT      BSZ     1
0367 000447     041544          FSB     DEC     58.
     000450     000000
0368                            *
0369                            *  SUBROUTINE 3
0370                            *
0371 000451     0 12 000515     SUB3    IRS     IFLG
0372 000452     0 02 000437             LDA     NEXT
0373 000453     0 04 000455             STA     *+2
0374 000454     0 01 000456             JMP     *+2
0375 000455     0 000000                DAC     **
0376 000456    -0 10 000441             JST*    FAT
0377 000457     000003                  DEC     3
0378 000460     000000          D3      BSZ     1
0379 000461     000000          N       BSZ     1
0380 000462     000000          X       BSZ     1
0381 000463    -0 02 000460             LDA*    D3
0382 000464     140040                  SZE
0383 000465     0 01 000470             JMP     *+3
0384 000466     140040                  CKA
0385 000467     0 01 000471             JMP     *+2
0386 000470     140402                  OCT     140402          LDI
0387 000471     0 06 000512             ADD     ADWD
0388 000472     0 04 000514             STA     CH3+1
0389 000473    -0 10 000653             JST*    L22
0390 000474    -0 000461                DAC*    N
0391 000475    -0 10 000676             JST*    C21
0392 000476     0 01 000370             JMP     ERI
0393 000477     0 04 000513             STA     CH3
0394 000500    -0 10 000653             JST*    L22
0395 000501    -0 000462                DAC*    X
0396 000502    -0 10 000676             JST*    C21
0397 000503     0 01 000370             JMP     ERI
0398 000504     0415 77                 ALS     1
```

```
0399 000505   000201          IAB
0400 000506   0 02 000513     LDA   CH3
0401 000507   0410 04         LLL   12
0402 000510  -0 04 000514     STA*  CH3+1
0403 000511  -0 01 001600     JMP*  CL06
0404 000512   0 001472  ADWD DAC   WRD1
0405 000513   000000  CH3  BSZ   2
0406 000515   000000  IFLG BSZ   1
0407                        *
0408                        *  SUBROUTINE 4
0409                        *
0410 000516   0 12 000515  SUB4 IRS   IFLG
0411 000517   0 02 000437       LDA   NEXT
0412 000520   0 04 000522       STA   *+2
0413 000521   0 01 000523       JMP   *+2
0414 000522   0 000000          DAC   **
0415 000523  -0 10 000441       JST*  FAT
0416 000524   000003            DFC   3
0417 000525   000000       D4   BSZ   1
0418 000526   000000       I4   BSZ   1
0419 000527   000000       C    BSZ   1
0420 000530  -0 02 000525       LDA*  D4
0421 000531   100040            SZE
0422 000532   0 01 000535       JMP   *+3
0423 000533   140040            CLA
0424 000534   0 01 000536       JMP   *+2
0425 000535   140402            OCT   140402          LDI
0426 000536   0 06 000512       ADD   ADWD
0427 000537   0 04 000600       STA   CH4+1
0428 000540  -0 02 000526       LDA*  I4
0429 000541   101400            SMI
0430 000542   0 01 000546       JMP   *+4
0431 000543   140040            CLA
0432 000544  -0 04 000600       STA*  CH4+1
0433 000545  -0 01 001600       JMP*  CL06
0434 000546  -0 10 000653       JST*  L22
0435 000547  -0 000526          DAC*  I4
0436 000550  -0 10 000676       JST*  C21
0437 000551   0 01 000370       JMP   ERI
0438 000552   0 04 000602       STA   II4
0439 000553  -0 10 000653       JST*  L22
0440 000554  -0 000527          DAC*  C
0441 000555  -0 10 000676       JST*  C21
0442 000556   0 01 000370       JMP   ERI
0443 000557   000201            IAB
0444 000560   0 02 000602       LDA   II4
0445 000561   100400            SNZ
0446 000562   0 01 000570       JMP   *+6
0447 000563   0 07 000666       SUB   =1
0448 000564   000201            IAB
0449 000565   0415 76           ALS   2
0450 000566   000201            IAB
0451 000567   0 01 000561       JMP   *-6
0452 000570   000201            IAB
0453 000571   0 04 000601       STA   CH4+2
0454 000572   140401            CMA
0455 000573  -0 03 000600       ANA*  CH4+1
```

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0456 000574     0 05 000601         ERA   CH4+2
0457 000575    -0 04 000600         STA*  CH4+1
0458 000576    -0 01 016600         JMP*  CL06
0459 000577     000000      CH4     BSZ   3
0460 000602     000000      II4     BSZ   1
0461                        *
0462                        *  COUNTER INTERRUPTS
0463                        *     RESPONSE CODE
0464                        *
0465                        *
0466                        *       ICTR  ICT1,SET1,6,CTR1,FLG1,TIM1,ITM1,L
0467 000603     14 0570     ICT1 OCP   SET1
0468 000604     0 02 000426        LDA   CTRS+6
0469 000605     74 0570            OTA   SET1
0470 000606     0 01 000605        JMP   *-1
0471 000607     14 0470            OCP   CTR1
0472 000610     0 02 000622        LDA   FLG1
0473 000611     100040             SZE
0474 000612     0 01 000616        JMP   *+4
0475 000613     0 02 000061        LDA   '61
0476 000614     0 07 01474         SUB   TIM1
0477 000615     0 04 000623        STA   ITM1
0478 000616     0 12 000622        IRS   FLG1
0479 000617     000401             ENB
0480 000620     0 10 000042        JST   LNKB
0481 000621     0 01 000603        JMP   ICT1
0482 000622     000000      FLG1    BSZ   1
0483 000623     000000      ITM1    BSZ   1
0484                        *
0485                        *       ICTR  ICT2,SET2,8,CTR2,FLG2,TIM2,ITM2,L
0486 000624     14 0770     ICT2 OCP   SET2
0487 000625     0 02 000430        LDA   CTRS+8
0488 000626     74 0770            OTA   SET2
0489 000627     0 01 000626        JMP   *-1
0490 000630     14 0670            OCP   CTR2
0491 000631     0 02 000643        LDA   FLG2
0492 000632     100040             SZE
0493 000633     0 01 000637        JMP   *+4
0494 000634     0 02 000061        LDA   '61
0495 000635     0 07 01475         SUB   TIM2
0496 000636     0 04 000644        STA   ITM2
0497 000637     0 12 000643        IRS   FLG2
0498 000640     000401             ENB
0499 000641     0 10 000055        JST   LNKC
0500 000642     0 01 000624        JMP   ICT2
0501 000643     000000      FLG2    BSZ   1
0502 000644     000000      ITM2    BSZ   1
0503                        *
0504                        *       ICTR  ICT3,SET3,10,CTR3,FLG3,TIM3,ITM3,
0505 000645     14 0370     ICT3 OCP   SET3
0506 000646     0 02 000432        LDA   CTRS+10
0507 000647     74 0370            OTA   SET3
0508 000650     0 01 000647        JMP   *-1
0509 000651     14 0270            OCP   CTR3
0510 000652     0 02 000664        LDA   FLG3
0511 000653     100040             SZE
0512 000654     0 01 000660        JMP   *+4
```

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0513 000655   0 02 000061        LDA   '61
0514 000656   0 07 001476        SUB   TIM3
0515 000657   0 04 000665        STA   ITM3
0516 000660   0 12 000664        IRS   FLG3
0517 000661   040401             ENB
0518 000662   0 10 000670        JST   LNRD
0519 000663   0 01 000645        JMP   ICT3
0520 000664   000000      FLG3  BSZ   1
0521 000665   000000      ITM3  BSZ   1
0522 000666   000001            FIN
     000667   000010
     000670   000004
     000671   000002
     000672   177763
     000673   000012
     000674   177773

0523          000675      BAS1  EQU   *
0524                      *
0525                      *  CLOCK INTERRUPT RESPONSE CODE
0526                      *
0527                            ORG   '1000
0528                            SETB  BAS2
0529 001000   14 002200  ACLK  OCP   SCLK
0530 001001   0 02 000440        LDA   CINT
0531 001002   0 04 000061        STA   '61
0532 001003   14 000200          OCP   CLK
0533 001004   040401            ENB
0534 001005   0 02 000024        LDA   LNKA+5
0535 001006   0 07 001466        SUB   BSTP
0536 001007   100400            SPL
0537 001010   0 01 001604        JMP   STP
0538 001011   0 02 000515        LDA   IFLG
0539 001012   100040            SZE
0540 001013   0 01 001604        JMP   STP
0541 001014   0 12 000515        IRS   IFLG
0542                      *
0543                      *  COUNTER INPUTS
0544                      *
0545                      *
0546                      *       CTR1  =2,A3,CTR1,TIM1,6,SET1,=48,ITM1,F
0547 001015   041001            INH
0548 001016   0 02 000420        LDA   CTRS
0549 001017   0 03 001637        ANA   =2
0550 001020   101040            SNZ
0551 001021   0 01 001064        JMP   A3
0552 001022   140040            CRA
0553 001023   54 000470         INA   CTR1
0554 001024   0 01 001023        JMP   *-1
0555 001025   000201            IAB
0556 001026   0 02 000061        LDA   '61
0557 001027   0 04 001474        STA   TIM1
0558 001030   0 02 000426        LDA   CTRS+6
0559 001031   74 000570         OTA   SET1
0560 001032   0 01 001031        JMP   *-1
0561 001033   000401            ENB
0562 001034   0 02 000242        LDA   PARS+1
```

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0563 01035   0 06 01636        ADD   =48
0564 01036   0 06 01636        ADD   =48
0565 01037   0 04 01055        STA   **14
0566 01040   140442            OCT   140442          A2A
0567 01041   0 04 01047        STA   **6
0568 01042   140442            OCT   140442          A2A
0569 01043   0 04 01061        STA   **14
0570 01044   000201            IAB
0571 01045  -0 10 00675        JST*  C12
0572 01046  -0 10 00654        JST*  H22
0573 01047   0 000000          DAC   **
0574 01050   0 02 00623        LDA   ITM1
0575 01051  -0 10 00675        JST*  C12
0576 01052  -0 10 00670        JST*  D22
0577 01053   0 001447          DAC   F50
0578 01054  -0 10 00654        JST*  H22
0579 01055   0 000000          DAC   **
0580 01056   0 02 00622        LDA   FLG1
0581 01057  -0 10 00675        JST*  C12
0582 01060  -0 10 00654        JST*  H22
0583 01061   0 000000          DAC   **
0584 01062   140040            CRA
0585 01063   0 04 00622        STA   FLG1
0586 01064   000401        A3  ENB
0587                       *
0588                       *    CTRI  =4,A4,CTR2,TIM2,8,SET2,=51,TIM2,F
0589 01065   000201            INB
0590 01066   0 02 00420        LDA   CTRS
0591 01067   0 03 01635        ANA   =4
0592 01070   101040            SNZ
0593 01071   0 01 01134        JMP   A4
0594 01072   140040            CRA
0595 01073   54 0670           INA   CTR2
0596 01074   0 01 01073        JMP   *-1
0597 01075   000201            IAB
0598 01076   0 02 00061        LDA   '61
0599 01077   0 04 01475        STA   TIM2
0600 01100   0 02 00430        LDA   CTRS+8
0601 01101   74 0770           OTA   SET2
0602 01102   0 01 01101        JMP   *-1
0603 01103   000401            ENB
0604 01104   0 02 00242        LDA   PARS+1
0605 01105   0 06 01634        ADD   =51
0606 01106   0 06 01634        ADD   =51
0607 01107   0 04 01125        STA   **14
0608 01110   140442            OCT   140442          A2A
0609 01111   0 04 01117        STA   **6
0610 01112   140442            OCT   140442          A2A
0611 01113   0 04 01131        STA   **14
0612 01114   000201            IAB
0613 01115  -0 10 00675        JST*  C12
0614 01116  -0 10 00654        JST*  H22
0615 01117   0 000000          DAC   **
0616 01120   0 02 00644        LDA   ITM2
0617 01121  -0 10 00675        JST*  C12
0618 01122  -0 10 00670        JST*  D22
0619 01123   0 001447          DAC   F50
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0420 01124  -0 10 00654          JST*  H22
0421 01125   0 000000            DAC   **
0422 01126   0 02 00643          LDA   FLG2
0423 01127  -0 10 00675          JST*  C12
0424 01130  -0 10 00654          JST*  H22
0425 01131   0 000000            DAC   **
0426 01132   140040              CRA
0427 01133   0 04 00643          STA   FLG2
0428 01134   000401        A4    ENB
0429                       *
0430                       *
0431 01135   001001        *     CTR1  =8,A5,CTR3,TIM3,10,SET3,=54,TIM3,
0432 01136   0 02 00420          INH
0433 01137   0 03 01633          LDA   CTRS
0434 01140   101040              ANA   =8
0435 01141   0 01 01204          SNZ
0436 01142   140040              JMP   A5
0437 01143   54 0270             CRA
0438 01144   0 01 01143          INA   CTR3
0439 01145   000201              JMP   *-1
0440 01146   0 02 00061          IAB
0441 01147   0 04 01476          LDA   '61
0442 01150   0 02 00432          STA   TIM3
0443 01151   74 0370             LDA   CTRS+10
0444 01152   0 01 01151          OTA   SET3
0445 01153   000401              JMP   *-1
0446 01154   0 02 00242          ENB
0447 01155   0 06 01632          LDA   PARS+1
0448 01156   0 06 01632          ADD   =54
0449 01157   0 04 01175          ADD   =54
0450 01160   140442              STA   **+14
0451 01161   0 04 01167          OCT   140442                A2A
0452 01162   140442              STA   **+6
0453 01163   0 04 01201          OCT   140442                A2A
0454 01164   000201              STA   **+14
0455 01165  -0 10 00675          IAB
0456 01166  -0 10 00654          JST*  C12
0457 01167   0 000000            JST*  H22
0458 01170   0 02 00665          DAC   **
0459 01171  -0 10 00675          LDA   TIM3
0460 01172  -0 10 00670          JST*  C12
0461 01173   0 000447            JST*  D22
0462 01174  -0 10 00654          DAC   F50
0463 01175   0 000000            JST*  H22
0464 01176   0 02 00664          DAC   **
0465 01177  -0 10 00675          LDA   FLG3
0466 01200  -0 10 00654          JST*  C12
0467 01201   0 000000            JST*  H22
0468 01202   140040              DAC   **
0469 01203   0 04 00664          CRA
0470 01204   000401        A5    STA   FLG3
0471                       *     ENB
0472                       *
0473                       *  DIGITAL OUTPUTS
0474                       *
0475                       *
0476                       *     DIGO  =64,A6,11,=89,LOOP,LAB1,DGP1,DGO1
0476 01205   0 02 00420          LDA   CTRS
```

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0477 01206     0 03 01631          ANA   =64
0478 01207     101040              SNZ
0479 01210     0 01 01244          JMP   A6
0480 01211     0 02 00433          LDA   CTRS+11
0481 01212     0 11 01630          CAS   =1
0482 01213   - 0 10 01603          JST*  SPSR
0483 01214     0 01 01241          JMP   DGO1
0484 01215     0 02 00242          LDA   PARS+1
0485 01216     0 06 01627          ADD   =89
0486 01217     0 06 01627          ADD   =89
0487 01220     0 04 01467          STA   LOCR
0488 01221     140040              CRA
0489 01222     0 04 01472          STA   WRD1
0490 01223     0 35 01626          LDX   =-16
0491 01224     0 02 01472 DGR1     LDA   WRD1
0492 01225     0415 77             ALS   1
0493 01226     0 04 01472          STA   WRD1
0494 01227   - 0 02 01467          LDA*  LOCR
0495 01230     101040              SNZ
0496 01231     0 01 01235          JMP   *+4
0497 01232     0 02 01472          LDA   WRD1
0498 01233     141006              AOA
0499 01234     0 04 01472          STA   WRD1
0500 01235     0 12 01467          IRS   LOCR
0501 01236     0 12 01467          IRS   LOCR
0502 01237     0 12 00000          IRS   0
0503 01240     0 01 01224          JMP   DGR1
0504 01241     0 02 01472 DGO1     LDA   WRD1
0505 01242     74 1370             OTA   DGOA
0506 01243     0 01 01242          JMP   *-1
0507                       *
0508                       *       DIGO  =128,A7,12,=165,LOCR+1,WRD2,DGR2
0509 01244                 A6      BSS   0
0510 01244     0 02 00420          LDA   CTRS
0511 01245     0 03 01625          ANA   =128
0512 01246     101040              SNZ
0513 01247     0 01 01303          JMP   A7
0514 01250     0 02 00434          LDA   CTRS+12
0515 01251     0 11 01630          CAS   =1
0516 01252   - 0 10 01603          JST*  SPSR
0517 01253     0 01 01300          JMP   DGO2
0518 01254     0 02 00242          LDA   PARS+1
0519 01255     0 06 01624          ADD   =165
0520 01256     0 06 01624          ADD   =165
0521 01257     0 04 01470          STA   LOCR+1
0522 01260     140040              CRA
0523 01261     0 04 01473          STA   WRD2
0524 01262     0 35 01626          LDX   =-16
0525 01263     0 02 01473 DGR2     LDA   WRD2
0526 01264     0415 77             ALS   1
0527 01265     0 04 01473          STA   WRD2
0528 01266   - 0 02 01470          LDA*  LOCR+1
0529 01267     101040              SNZ
0530 01270     0 01 01274          JMP   *+4
0531 01271     0 02 01473          LDA   WRD2
0532 01272     141006              AOA
0533 01273     0 04 01473          STA   WRD2
```

```
0734 01274    0 12 01470          IRS   LOCK+1
0735 01275    0 12 01470          IRS   LOCK+1
0736 01276    0 12 00000          IRS   0
0737 01277    0 01 01263          JMP   DGK2
0738 01300    0 02 01473 DGO2     LDA   WRD2
0739 01301    74 1270             OTA   DGOR
0740 01302    0 01 01301          JMP   *-1
0741                      *
0742                      *  ANALOGUE INPUTS SCAN
0743                      *
0744                      *
0745                      *       DVCF  =1,AK
0746 01303                A7    RSS   0
0747 01303    0 02 00420          LDA   CTKS
0748 01304    0 03 01630          ANA   =1
0749 01305    1F1040              SNZ
0750 01306    0 01 01477          JMP   AB
0751 01307    0 35 01623          LDX   =-4K
0752 01310    140640              CKA
0753 01311   -0 04 01352          STA*  AB4K
0754 01312    0 12 00000          IRS   0
0755 01313    0 01 01311          JMP   *-2
0756 01314    0 02 00424          LDA   CTKS+4
0757 01315    140407              TCA
0758 01316    0 04 01435          STA   ENS
0759 01317    0 02 00423          LDA   CTKS+3
0760 01320    0 06 01353          ADD   AB4K+1
0761 01321    0 04 01354          STA   AB4K+2
0762 01322    0 02 00423          LDA   CTKS+3
0763 01323    0 07 00422          SUB   CTKS+2
0764 01324    141006              AOA
0765 01325    140407              TCA
0766 01326    0 04 01471          STA   CHXN
0767 01327    0 35 01471 ESBL     LDX   CHXN
0768 01330    0 02 00422          LDA   CTKS+2
0769 01331    0 04 01436          STA   STOP
0770 01332    0 02 01436 MUX      LDA   STOP
0771 01333    74 0170             OTA   ANAG
0772 01334    0 01 01333          JMP   *-1
0773 01335    14 00076            OCP   DATA
0774 01336    140040              CKA
0775 01337    54 00076            INA   DATA
0776 01340    0 01 01337          JMP   *-1
0777 01341    04014 72            LGR   6
0778 01342   -0 06 01354          ADD*  AB4K+2
0779 01343   -0 04 01354          STA*  AB4K+2
0780 01344    0 12 01436          IRS   STOP
0781 01345    0 12 00000          IRS   0
0782 01346    0 01 01332          JMP   MUX
0783 01347    0 12 01435          IRS   ENS
0784 01350    0 01 01327          JMP   ESBL
0785 01351    0 01 01437          JMP   A7A
0786 01352    1 01 1435     AB4K  DAC   ABUF+4K,1
0787 01353    1 001356            DAC   ABUF+1,1
0788 01354    000000              BSZ   1
0789 01355    000000        ABUF  BSZ   4K
0790 01435    000000        ENS   BSZ   1
```

```
0791 01436   000000          STUP BSZ   1
0792                         *
0793                         * ANALOGUE DATA PROCESSING
0794                         *
0795 01437   0 02 00422  A7A  LDA   CTRS+2
0796 01440   0 06 01463       ADD   BF
0797 01441   0 04 01464       STA   ADBF
0798 01442   0 02 00242       LDA   PARS+1
0799 01443   0 06 00422       ADD   CTRS+2
0800 01444   0 06 00422       ADD   CTRS+2
0801 01445   0 04 01465       STA   DBF
0802 01446   0 35 01471       LDX   CHXR
0803 01447  -0 02 01464  REP  LDA*  ADBF
0804 01450  -0 10 00675       JST*  C12
0805 01451  -0 10 00670       JST*  D22
0806 01452   0 000000         DAC   **
0807 01453  -0 10 00654       JST*  H22
0808 01454. -0 001465         DAC*  DBF
0809 01455   0 12 01464       IRS   ADBF
0810 01456   0 12 01465       IRS   DBF
0811 01457   0 12 01465       IRS   DBF
0812 01460   0 12 000000      IRS   0
0813 01461   0 01 01447       JMP   REP
0814 01462   0 01 01477       JMP   A8
0815 01463   0 001355    BF   DAC   ABUF
0816 01464   000000      ADBF BSZ   1
0817 01465   000000      DBF  BSZ   1
0818 01466   0 000000    BSTP DAC   SKST
0819 01467   000000      LOCH BSZ   2
0820 01471   000000      CHXR BSZ   1
0821 01472   000000      WRD1 BSZ   1
0822 01473   000000      WRD2 BSZ   1
0823 01474   000000      TIM1 BSZ   1
0824 01475   000000      TIM2 BSZ   1
0825 01476   000000      TIM3 BSZ   1
0826                         *
0827                         * DIGITAL INPUTS
0828                         *
0829                         *
0830                         *     DIGI  =16,A9,DGIA,=57,DGS1,DGT1
0831 01477                   A8    BSS   0
0832 01477   0 02 00420       LDA   CTRS
0833 01500   0 03 01640       ANA   =16
0834 01501   101040          SNZ
0835 01502   0 01 01533       JMP   A9
0836 01503   54 1170          INA   DGIA
0837 01504   0 01 01503       JMP   *-1
0838 01505   0 04 01602       STA   HOLD
0839 01506   0 35 01626       LDX   =-16
0840 01507   0 02 00242       LDA   PARS+1
0841 01510   0 06 01622       ADD   =57
0842 01511   0 06 01622       ADD   =57
0843 01512   0 04 01526       STA   DGS1
0844 01513   140040          CRA
0845 01514   000201          IAB
0846 01515   0 02 01602  DGT1 LDA   HOLD
0847 01516   0416 77          ALR   1
```

```
0848 01517   0 04 01602        STA   HOLD
0849 01520   101001            SSC
0850 01521   0 01 01524        JMP   *+3
0851 01522   0 02 01621        LDA   ='40300
0852 01523   0 01 01525        JMP   *+2
0853 01524   140040            CRA
0854 01525  -0 10 00654        JST*  H22
0855 01526   0 000000    DGS1  DAC   **
0856 01527   0 12 01526        IRS   DGS1
0857 01530   0 12 01526        IRS   DGS1
0858 01531   0 12 00000        IRS   0
0859 01532   0 01 01515        JMP   DGT1
0860                          *
0861                          *     DIGI  =32,A10,DGIB,=73,DGS2,DGT2
0862 01533                    A9    BSS   0
0863 01533   0 02 00420        LDA   CTRS
0864 01534   0 03 01620        ANA   =32
0865 01535   101040            SNZ
0866 01536   0 01 01567        JMP   A10
0867 01537   54 1070          INA   DGIB
0868 01540   0 01 01537        JMP   *-1
0869 01541   0 04 01602        STA   HOLD
0870 01542   0 35 01626        LDX   =-16
0871 01543   0 02 00242        LDA   PARS+1
0872 01544   0 06 01617        ADD   =73
0873 01545   0 06 01617        ADD   =73
0874 01546   0 04 01562        STA   DGS2
0875 01547   140040            CRA
0876 01550   000201            IAB
0877 01551   0 02 01602  DGT2  LDA   HOLD
0878 01552   0416 77          ALR   1
0879 01553   0 04 01602        STA   HOLD
0880 01554   101001            SSC
0881 01555   0 01 01560        JMP   *+3
0882 01556   0 02 01621        LDA   ='40300
0883 01557   0 01 01561        JMP   *+2
0884 01560   140040            CRA
0885 01561  -0 10 00654        JST*  H22
0886 01562   0 000000    DGS2  DAC   **
0887 01563   0 12 01562        IRS   DGS2
0888 01564   0 12 01562        IRS   DGS2
0889 01565   0 12 00000        IRS   0
0890 01566   0 01 01551        JMP   DGT2
0891                          *
0892                          * UPDATE SCANS DONE
0893                          *
0894 01567   0 12 01601  A10   IRS   SCAN
0895                          *
0896                          *     REST  SIP1,SBP1
0897 01570   0 02 00442        LDA   SIP1
0898 01571   0 04 00034        STA   SIP
0899 01572   0 02 00443        LDA   SBP1
0900 01573   0 04 00037        STA   SBP
0901 01574   0 02 01600        LDA   CL06
0902 01575   0 04 00204        STA   GOAD
0903                          *
0904                          *     RETN  LNRA,ACLK
```

```
0905 01576    0 10 00027        JST   LNRA
0906 01577    0 01 01000        JMP   ACLK
0907 01000    004013      CL06  OCT   4013
0908 01601    000000      SCAN  BSZ   1
0909 01602    000000      HOLD  BSZ   1
0910 01603    0 000000    SPSR  XAC   MYSR
0911 01604    0 10 01606  STP   JST   ERCL
0912 01605    152306            BCI   1,TF                SCAN TOO FAST
0913                      *
0914                      * ERROR RETURN TO BASIC
0915                      *
0916 01606    0 000000    ERCL  DAC   **
0917 01607   -0 02 01606        LDA*  ERCL
0918 01610    0 04 01616        STA   *+6
0919 01611    14 0220           OCP   SCLK
0920 01612    14 0570           OCP   SET1
0921 01613    14 0770           OCP   SET2
0922 01614    14 0370           OCP   SET3
0923 01615   -0 10 00163        JST*  ERR
0924 01616    0 000000          DAC   **
0925 01617    000111            FIN
     01620    000040
     01621    040300
     01622    000071
     01623    177720
     01624    000151
     01625    000200
     01626    177760
     01627    000131
     01630    000001
     01631    000100
     01632    000066
     01633    000010
     01634    000063
     01635    000004
     01636    000041
     01637    000002
     01640    000020

0926          001641      BAS2  EQU   *
0927                      *
0928                      *   PATCH IN BASIC
0929                      *  CALLING SEQUENCE
0930                      *
0931                            ABS
0932                            ORG   '4012
0933 04012   -0 01 00716        JMP*  '716
0934                            ORG   '716
0935 00716    0 000211          DAC   CALL
0936                            ORG   '551
0937 00551    0 001606          DAC   ERCL
0938                            END

A1      000332    A10     001567    A2      000350    A3      001064
A4      001134    A5      001204    A6      001244    A7      001303
A7A     001437    A8      001477    A9      001533    AB48    001352
ABUF    001355    ACLK    001000    ADBF    001464    ADWD    000512
```

ANAG	000170A	BAS1	000675	BAS2	001641	BF	001463
BSTP	001466	C	000527	C12	00067SA	C21	00067GA
CALL	000211	CH3	000513	CH4	000577	CHXR	001471
CIH	000073	CIHA	000117	CII	000143	CIN1	000440
CIR	000120	CIRA	000160	CIRX	000161	CJST	00051SA
CLK6	001600	CLK	000020A	CONT	000007	CTR1	000470A
CTR2	000670A	CTR3	000270A	CTRS	000420	D22	000670A
D3	000460	D4	000525	DACS	000435	DATA	000070A
DBF	001465	DGIA	001170A	DGIB	001070A	DGO1	001241
DGO2	001300	DGOA	001370A	DGOB	001270A	DGR1	001224
DGR2	001263	DGS1	001526	DGS2	001562	DGT1	001515
DGT2	001551	DISP	000164	DISQ	000177	DISS	000203
ENS	001435	ERCL	001606	ERI	000370	ERR	000163
ESRL	001327	F50	000447	FAT	000441	FLG1	000622
FLG2	000643	FLG3	000664	FRST	000436	GOAD	000204
H22	00065AA	HAD	001770A	HOLD	001602	I4	000526
IBUF	000230A	ICT1	000603	ICT2	000624	ICT3	000645
IFLG	000515	II4	000602	INT	000366	ITM1	000623
ITM2	000644	ITM3	000665	KT	000446	L22	00065JA
LNKA	000017	LNKB	000032	LNKC	000045	LNKD	000060
LNRA	000027	LNRB	000042	LNRC	000055	LNRD	000070
LOCB	001467	M22	000674A	MASK	000162	MUX	001332
N	000461	NEXT	000437	PARS	000241	REP	001447
SBP	000037A	SBP1	000443	SBP2	000445	SCAN	001601
SCLK	000220A	SET1	000570A	SET2	000770A	SET3	000370A
SIP	000034A	SIP1	000442	SIP2	000444	SKST	000000
SPSR	001603	SS	004064A	STOP	000175	STP	001604
STUP	001436	SUB1	000227	SUB2	000372	SUB3	000451
SUB4	000516	TABL	000215	TIM1	001474	TIM2	001475
TIM3	001476	WRD1	001472	WRD2	001473	X	000462

0000 WARNING OR ERROR FLAGS
DAP-16 MOD 2 REV. C 01-26-71

```
*LOW    00551
*START  00551
*HIGH   37743
*NAMES  12773
*COMN   37777
*BASE   37671
*BASF   36704
RADIOS  36000
IFLG    36515
ESAT    36710
RRCL    37606
MYSR    37700
TOMOD   37710

LC
```

```
                                * SUBROUTINE 5  3.05.78        PAGE    1


                                * SUBROUTINE 5  3.05.78
0001                            *
0002                                    REL
0003
0004            000653      L22 EQU     '653
0005            000676      C21 EQU     '676
0006            001370      DGOA EQU    '1370
0007            001270      DGOB EQU    '1270
0008                                    SUBR  SUBS
0009 00000      0 000000    SUBS DAC    **
0010 00001     -0 10 00034          JST*  FAT
0011 00002      000003              DEC   3
0012 00003      000000      DS      BSZ   1
0013 00004      000000      NS      BSZ   1
0014 00005      000000      XS      BSZ   1
0015 00006     -0 12 00035          IRS*  FLAG
0016 00007     -0 10 00653          JST*  L22
0017 00010     -0 000004            DAC*  NS
0018 00011     -0 10 00676          JST*  C21
0019 00012     -0 01 00033          JMP*  ERI
0020 00013      0 04 00036          STA   CH3
0021 00014     -0 10 00653          JST*  L22
0022 00015     -0 000005            DAC*  XS
0023 00016     -0 10 00676          JST*  C21
0024 00017     -0 01 00033          JMP*  ERI
0025 00020      0415 77             ALS   1
0026 00021      000201              IAB
0027 00022      0 02 00036          LDA   CH3
0028 00023      0400 74             LRL   4
0029 00024     -0 02 00003          LDA*  DS
0030 00025      100040              SZE
0031 00026      0 01 00033          JMP   *+5
0032 00027      000201              IAB
0033 00030      74 1370             OTA   DGOA
0034 00031      0 01 00030          JMP   *-1
0035 00032     -0 01 00000          JMP*  SUBS
0036 00033      036370      ERI     OCT   36370
0037 00034      036710      FAT     OCT   36710
0038 00035      036515      FLAG    OCT   36515
0039 00036      000000      CH3     BSZ   1
0040                                    END

C21     000676A   CH3     000036   DS      000003   DGOA    001370A
DGOB    001270A   ERI     000033   FAT     000034   FLAG    000035
L22     000653A   NS      000004   SUBS    000000   XS      000005

0000 WARNING OR ERROR FLAGS
DAP-16 MOD 2    REV. C    01-26-71
```

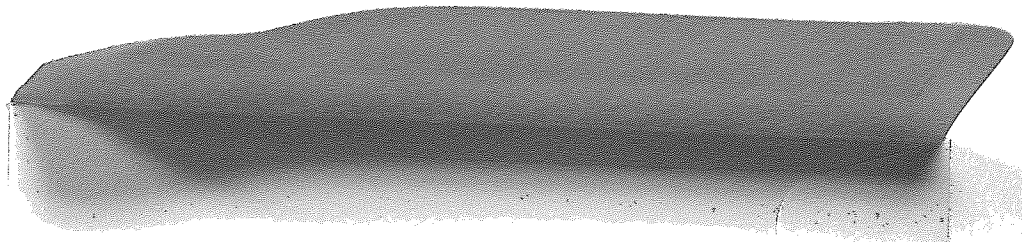
```
        ABS
        ORG     '37347
        JMP     PCH2
        ORG     '37326
        JMP     PCH1
        ORG     '37743
PCH1    STA     CHXR
        CRA
        STA     ENS
        LDA     '61
        STA     XREG
        LDA     '61
        STA     SAVE
        ERA     XREG
        SNZ
        JMP     *-4
        JMP     ESBL
PCH2    IRS     ENS
        LDA     '61
        ERA     SAVE
        SNZ
        JMP     DLY
        LDA     ENS
        JST*    C12
        JST*    H22
        DAC*    REP+3
        JMP     A7A
DLY     LDA     CTS
        STA     XREG
        IRS     XREG
        JMP     *-1
        JMP     ESBL
SAVE    BSZ     1
CTS     BSZ     1
XREG    BSZ     1
CHXR    EQU     '37471
ENS     EQU     '37435
C12     EQU     '675
H22     EQU     '654
REP     EQU     '37447
A7A     EQU     '37437
ESBL    EQU     '37327
        END
```

APPENDIX E

E.1 Listings of the Open-Loop Estimation Package (EKF3)

The Contents of the Microfiche

Frame A1	: the contents
Frames A1,B1,.....O1 A2,B2,.....O2 A3,B3,.....O3 A4,B4,C4	: simulated open-loop estimation results when the column is subjected to multiple changes in the feed rate, composition and temperature. Zero mean White Gaussian noise is added to the measurements. Sample time is 18 seconds.



APPENDIX F

F.1 Listings of the EAFF Control Package

The Contents of the Microfiche

Frame A1 : the contents

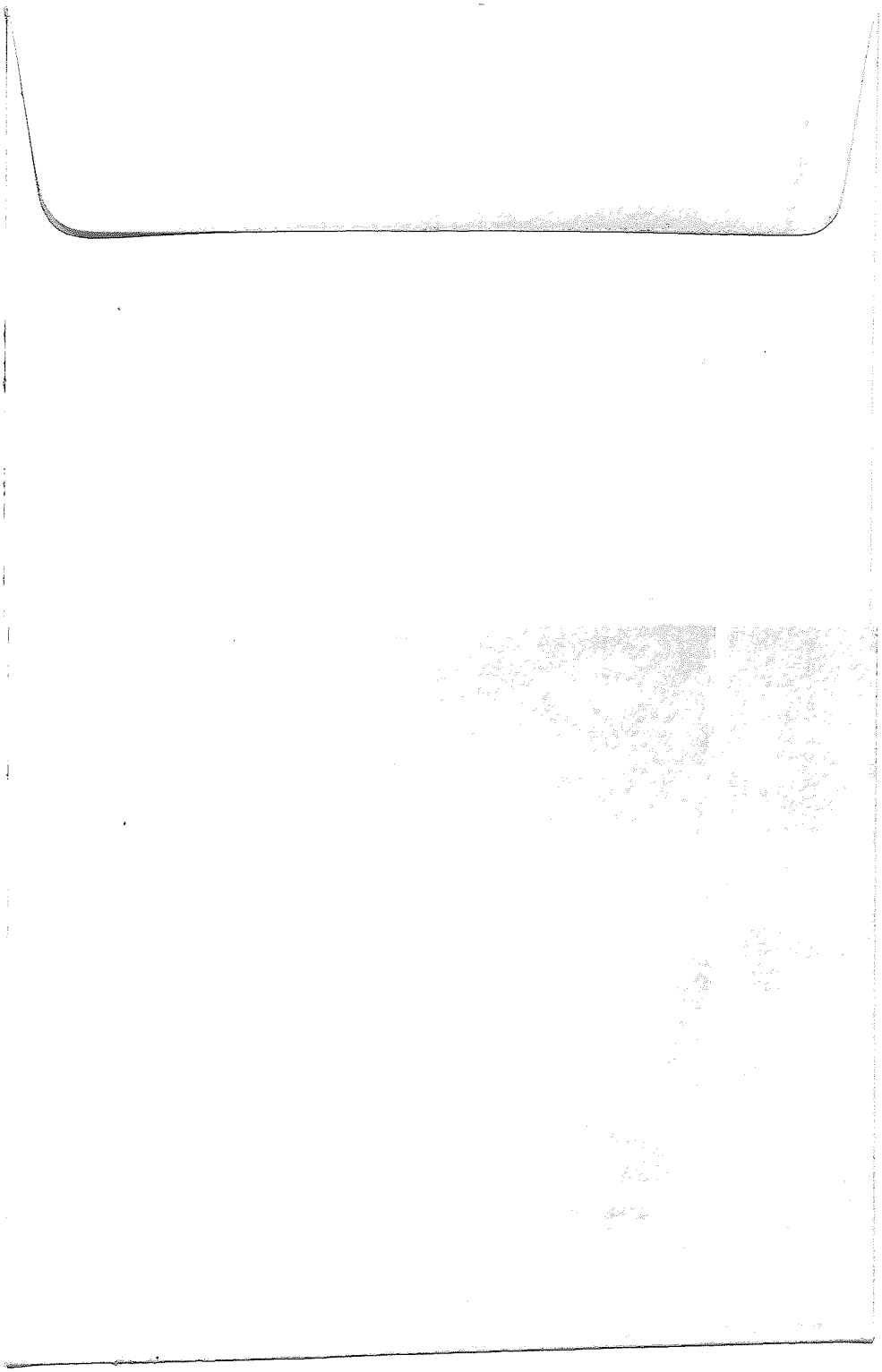
Frames A1,B1,.....O1 : listings of the EAFF control
A2,B2,.....O2 simulation package
A3,B3,.....O3
A4,B4,C4,D4,E4

Frames E4 to F4 : the simulated column response to a single step increase in the feed rate under EAFF control. The measurements are corrupted by zero mean White Gaussian noise. Sample time is 18 seconds.

Frames F9 to G14 : the simulated column response to multiple changes in the feed rate, composition and temperature under EAFF control. The measurements are corrupted by zero mean White Gaussian noise. Sample time is 18 seconds.

Frames G14 onwards : the simulated column response to multiple step changes in the feed rate, composition and

tempearture under EAFF control. The measurements are corrupted by zero mean White Gaussian noise. Sample time is increased to 25 seconds.



APPENDIX G

The equilibrium relationship used in the model is

$$y_i = \frac{\alpha_i P_i^{\circ}(T)}{P} x_i$$

or $y_i = K_i x_i$; where $K_i = g(x_i)$

Thus this functional relationship can be included as follows:

$$f_i = \frac{L_{i-1}(x_{i-1} - x_i) + V(y_{i+1} - K_i x_i)}{M_i}$$

Thus, if we assume $\frac{\partial K_i}{\partial x_i}$ to be negligible, the modified elements of the state transition matrix would be

Row 1	$\frac{\partial f_i}{\partial x_j} = -\frac{(L_R + VK_1)}{M_1}$	j=1 only
Rows 1 to 6	$\frac{\partial f_i}{\partial x_j} = -\frac{(L_{i-1} + VK_i)}{M_i}$	i=1,6; j=i only
Row 7	$\frac{\partial f_7}{\partial x_j} = -\frac{(L_6 + F + VK_7)}{M_7}$	j=7 only
Rows 8 to 10	$\frac{\partial f_i}{\partial x_j} = -\frac{(L_{i-1} + VK_i)}{M_i}$	i=8,10; j=i only
Row 11	$\frac{\partial f_{11}}{\partial x_j} = -\frac{L_{10} + V - K_{11}V}{M_{11}}$	j=11 only

NOTATION

Chapter II

$\underline{A}$ = relating matrix

$\underline{B}$ = the matrix of left eigen vectors of $\underline{A}$

B = bottoms rate

B_1, B_2, B_3 = temperature measurements near the feed plate, an intermediate temperature and bottoms temperature respectively

$\underline{C}$ = the matrix of right eigen vectors of $\underline{A}$

C_p = molar specific heat capacity

D = distillate

$\underline{D}$ = driving matrix

F = feed rate

Z = feed composition

G_c = controller transfer function

G_v = valve transfer function

G_M = measurement transfer function

J = scalar performance criterion

$\underline{K}$ = proportional gain matrix

L_n = liquid leaving the nth tray

$\underline{P}$ = plant matrix or the Ricatti matrix

$\underline{Q}$ = positive semi definite weighting matrix

$\underline{R}$ = weighting matrix

R = reflux rate

R_I = internal reflux

S = separation factor

T_o = overhead temperature

T_r = reflux temperature

$\underline{u}_i$ = eigen vectors of $\underline{A}^T$

$\underline{u}(t)$ = control effort

$\underline{V}_i$ = eigen vectors of $\underline{A}$

V_n = vapour rate leaving the nth tray

x = liquid compositon

y = vapour composition

$\underline{X}$ = vector of state variables

Subscripts

m = measured value

Greek Symbols

λ_i = eigen values of $\underline{A}$

τ = hydraulic time constant

Filtering Notation

A = continuous matrix time function

D = continuous system input driving matrix

G = continuous matrix time function

K = filter gain matrix

$M(t)$ = continuous measurement matrix

$M(t_k)$ = discrete measurement matrix

P = error covariance matrix

Q = system noise covariance matrix

R = measurement noise covariance matrix

t = continuous time

t_k = discrete time

u = vector of deterministic system inputs

v = vector of white Gaussian noise

w = vector of random system disturbances represented by a zero mean white Gaussian process

x = vector of state variables

y = vector of measured variables

Greek symbols

β_t = vector of Brownian motion or Weiner process

Φ = state transition matrix

Γ = system noise coefficient matrix

Γ_D = discrete system input driving matrix

Chapter III

a,b,c,d,e = coefficients

C_p = specific heat capacity

M = mass of the liquid in the reboiler

M_B = reboiler holdup

M_D = reflux drum holdup

Q = heat transfer rate

Chapter IV

A = Brambilla equation constant

a = effective interfacial area for mass transfer

A_a = active area

B = Brambilla equation coefficient

C = Brambilla equation coefficient

C_p = specific heat capacity

C_1, C_2, C_3 = Antoine equation constants

D = distillate rate

D_E = eddy diffusivity

d_c = downcomer diameter

d_i = internal column diameter

D_ℓ = liquid diffusivity

D_v = vapour diffusivity

E_{mv} = Murphree tray efficiency

E_v = vaporization efficiency

E_{ov} = point efficiency

E_{oc} = overall column efficiency

E_n = Murphree vapour phase efficiency

F = feed rate

F_n = vapour flow parameter

f_i = fugacity of component i

f_i^{OL} = a standard state liquid fugacity

h, H = liquid and vapour enthalpies respectively

h_w = weir height

h_{ow} = liquid height over the weir

h_D = liquid height in the downcomer

h_f = froth height

h_ℓ = pressure drop through the aerated liquid

h_{hg} = hydraulic gradient across the plate

h_{ds} = calculated height of clear liquid over the disperser

K_ℓ = liquid phase transfer coefficient

L_n = liquid leaving the nth tray

L_o = bottoms rate

L_R = reflux rate

M_n = liquid holdup on the nth tray

M = molecular weight

M_D = reflux drum holdup

N_{ov} = number of overall mass transfer units

N_ℓ, N_v = liquid and vapour transfer units

N_{pe} = peclet number

N_{scg} = Schmidt number

P = total vapour pressure on a tray

P_c = total column pressure

$P_i^o(T)$ = saturation vapour pressure

Q = reboiler heat duty

q' = liquid flow rate

r = collision diameter

T = tray temperature

t = time

T_F = feed temperature

T^o = a reference temperature

T_r = reduced temperature

T_c = critical temperature

T_b = boiling point

U = the internal energy

U_a = vapour velocity through the active area

V_n = vapour leaving the nth tray

W = liquid flow rate or width of the flow path

x_n = liquid composition on the nth tray

Y_n = vapour composition

Z_c = critical compressibility

Z_ℓ = length of the liquid travel

Subscripts

c = critical value

b = boiling point

m = mixture

G = vapour phase

i,j,n = refer to the ith, the jth and the nth components

ℓ = liquid

Superscripts

L = liquid phase

V = vapour phase

Greek Symbols

γ = activity coefficient

λ = latent heat of vaporization

ψ = fugacity coefficient

Φ = average relative froth density on the tray

ρ = density

μ = viscosity

θ = residence time of liquid in the froth zone

β = aeration factor

Chapter VI

The symbols are identical with the notations for filtering in Chapter II. Additionally the following notation are also used.

$\bar{x}$ = the estimated value of x

$\hat{x}$ = the predicted value of x

Chapter VII

I = the identity matrix

x_j = state variables in the filters

x_n = the liquid composition on a tray

M_n = the liquid holdup on a tray

M = measurement matrix

δ_i = the elements of the jacobian

L_i = liquid rate leaving each tray

v = boilup rate

y = actual vapour composition in mass balances
= measured variables in the filtering notation

x_F = feed composition

F = feed rate

LR = reflux rate

x_D = distillate composition

x_B = bottom composition

R = reflux rate
= measurement noise matrix in the filtering notation

P = the error covariance matrix

P = total pressure

P_i^o = saturation vapour pressure

P_i = vapour pressure

A_i, B_i, C_i = Antoine constants

T = temperature

Q = system noise covariance matrix

Chapter VIII

$\hat{\underline{x}}$ = estimated value of x

$\underline{x}_p$ = predicted value of x

$\underline{Y}$ = measurement vector

u = control effort

$\underline{K}$ = filter gain

IAE = integrated absolute error

LR = reflux rate

e = deviation from the set point

Q = heat input rate

x_i = composition

Subscripts

s = steady state bias

b = bottom loop

t = top loop

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